

Electronic Supplementary Information

Regulating and controlling the stepwise ESDPT channel of BP(OH)₂DCEt₂ with the strategy of solvent polarity and the external electric field

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Contents:

| | |
|---|-----|
| 1. Table S1. | S1 |
| 2. Table S2. | S1 |
| 3. Table S3. | S1 |
| 4. Figure S1. | S2 |
| 5. Figure S2. | S3 |
| 6. Table S4. | S3 |
| 7. Table S5. | S4 |
| 8. Table S6. | S4 |
| 9. Figure S3. | S5 |
| 10. Figure S4. | S5 |
| 11. Figure S5. | S6 |
| 12. Table S7. | S6 |
| 13. Figure S6. | S7 |
| 14. Figure S7. | S8 |
| 15. Figure S8. | S8 |
| 16. Table S8. | S9 |
| 17. Figure S9. | S9 |
| 18. Cartesian coordinates of all structures. | S10 |

Table S1. Obtained absorption, fluorescence peaks (including the enol and keto forms) and error (ΔE) between calculated values and experimental values of BP(OH)₂DCEt₂ by using different functions and basis sets in cyclohexane (CYH).

| | Abs. (nm) | | | DPT-Flu. (nm) | | |
|----------------------------|-------------------|------------|-----------------|-------------------|------------|-----------------|
| | Exp. ^a | Cal. | ΔE (eV) | Exp. ^a | Cal. | ΔE (eV) |
| Cam-B3LYP/6-311g (d, p) | 389 | 348 | 0.37 | 521 | 513 | 0.04 |
| wB97XD/6-311g (d, p) | 389 | 346 | 0.39 | 521 | 512 | 0.04 |
| B3LYP/6-311g (d, p) | 389 | 380 | 0.07 | 521 | 528 | 0.03 |
| B3LYP/6-311+g(d, p) | 389 | 381 | 0.06 | 521 | 529 | 0.04 |
| B3LYP/6-311++g(d, p) | 389 | 381 | 0.06 | 521 | 529 | 0.04 |

Table S2. Obtained absorption, fluorescence peaks (including the enol and keto forms) and error (ΔE) between calculated values and experimental values of BP(OH)₂DCEt₂ by using different functions and basis sets in dichloromethane (DCM).

| | Abs. (nm) | | | DPT-Flu. (nm) | | |
|----------------------------|-------------------|------------|-----------------|-------------------|------------|-----------------|
| | Exp. ^a | Cal. | ΔE (eV) | Exp. ^a | Cal. | ΔE (eV) |
| Cam-B3LYP/6-311g (d, p) | 389 | 347 | 0.38 | 521 | 517 | 0.02 |
| wB97XD/6-311g (d, p) | 389 | 345 | 0.4 | 521 | 516 | 0.02 |
| B3LYP/6-311g (d, p) | 388 | 379 | 0.08 | 521 | 531 | 0.05 |
| B3LYP/6-311+g(d, p) | 389 | 380 | 0.07 | 521 | 531 | 0.05 |
| B3LYP/6-311++g(d, p) | 389 | 380 | 0.07 | 521 | 531 | 0.05 |

Table S3. Obtained absorption, fluorescence peaks (including the enol and keto forms) and error (ΔE) between calculated values and experimental values of BP(OH)₂DCEt₂ by using different functions and basis sets in acetonitrile (ACN).

| | Abs. (nm) | | | DPT-Flu. (nm) | | |
|-------------------------|-------------------|------|-----------------|-------------------|------|-----------------|
| | Exp. ^a | Cal. | ΔE (eV) | Exp. ^a | Cal. | ΔE (eV) |
| Cam-B3LYP/6-311g (d, p) | 385 | 346 | 0.36 | 521 | 513 | 0.04 |

| | | | | | | |
|----------------------------|------------|------------|-------------|------------|------------|-------------|
| wB97XD/6-311g (d, p) | 385 | 343 | 0.39 | 521 | 512 | 0.04 |
| B3LYP/6-311g (d, p) | 385 | 377 | 0.07 | 521 | 527 | 0.03 |
| B3LYP/6-311+g(d, p) | 385 | 378 | 0.06 | 521 | 528 | 0.03 |
| B3LYP/6-311++g(d, p) | 385 | 378 | 0.06 | 521 | 528 | 0.03 |

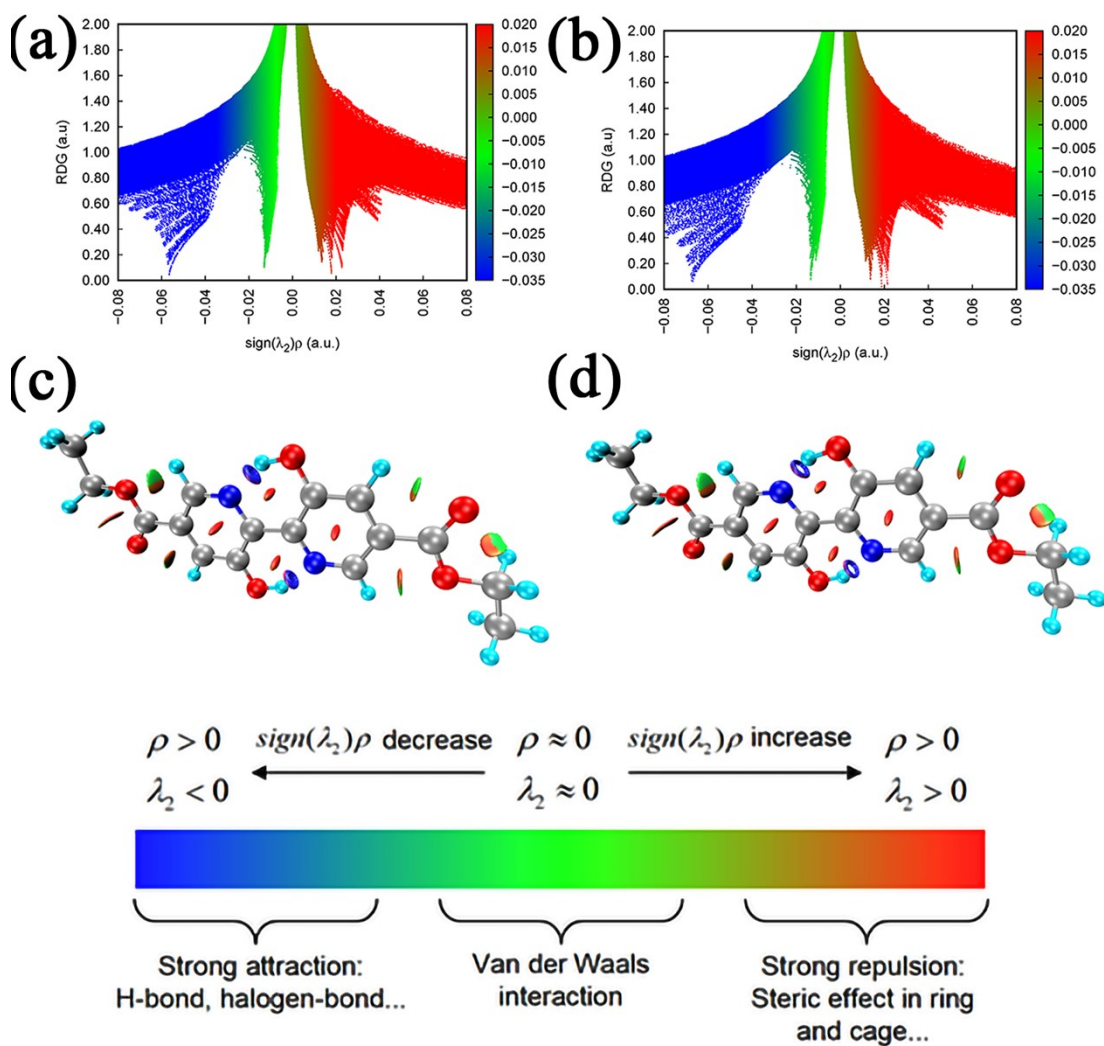


Figure S1. The scatter diagrams (top) of (a) S0 state and (b) S1 state, the RDG isosurfaces (bottom) of (c) S0 state and (d) S1 state in CYH solvent.

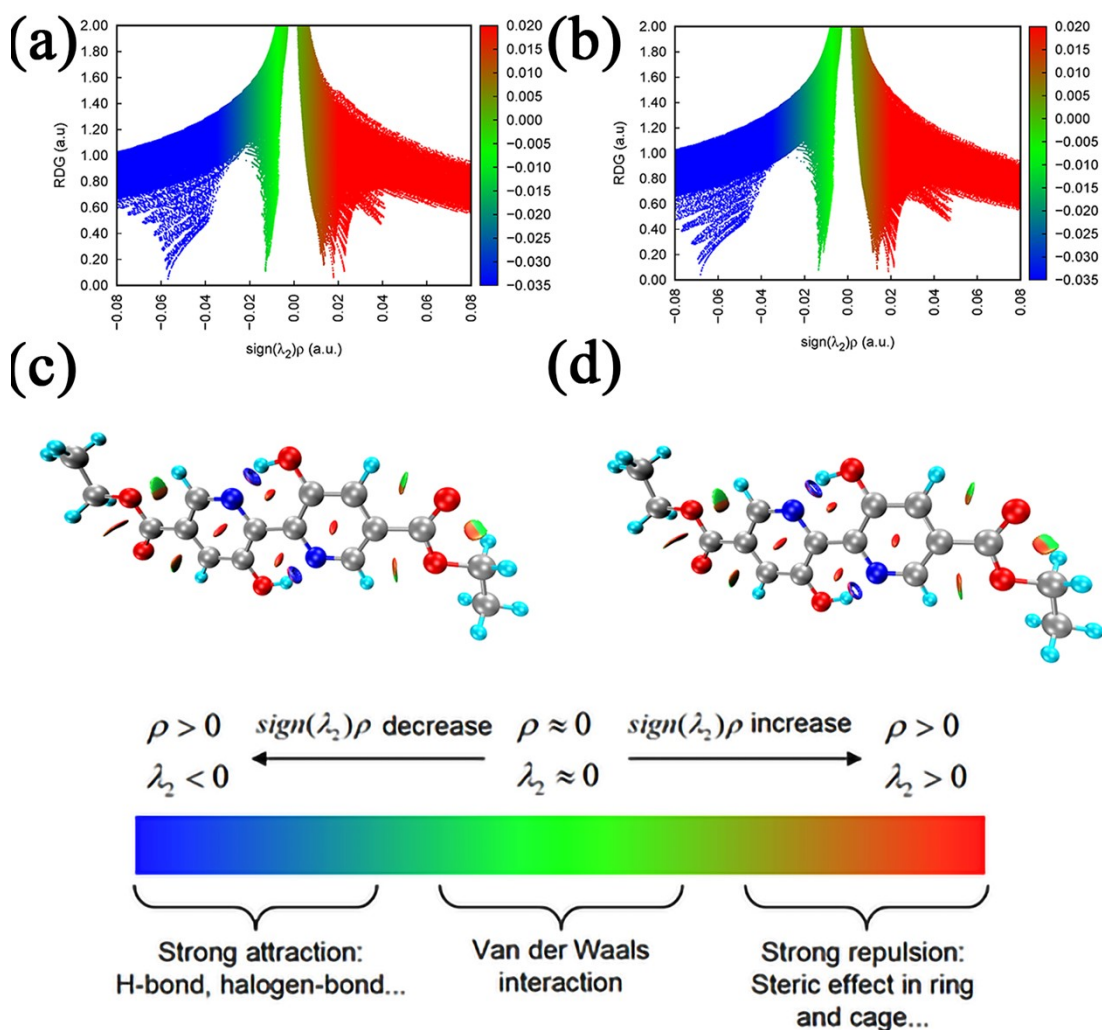


Figure S2. The scatter diagrams (top) of (a) S0 state and (b) S1 state, the RDG isosurfaces (bottom) of (c) S0 state and (d) S1 state in DCM solvent.

Table S4. Electronic excitation energy (nm), corresponding oscillator strengths (a.u.), and the transition percentage (%) for BP(OH)₂DCEt₂ system in ACN, DCM and CYH solvents.

| | Transition | λ | f | composition | CI(%) |
|-----|------------|-----------|--------|-------------|--------|
| ACN | S0→S1 | 377 | 0.6526 | H→L | 98.70% |
| | S0→S2 | 316 | 0.0008 | H-2→L | 97.60% |
| | S0→S3 | 299 | 0.0000 | H-1→L | 92.90% |
| DCM | S0→S1 | 379 | 0.6675 | H→L | 98.80% |

| | | | | | |
|-----|-------|-----|--------|-------|--------|
| | S0→S2 | 317 | 0.0008 | H-2→L | 97.60% |
| | S0→S3 | 300 | 0.0000 | H-1→L | 93.10% |
| | S0→S1 | 380 | 0.6572 | H→L | 98.80% |
| CYH | S0→S2 | 318 | 0.0008 | H-2→L | 97.50% |
| | S0→S3 | 300 | 0.0000 | H-1→L | 93.00% |

Table S5. Electronic emission energy (nm), corresponding oscillator strengths (a.u.), and the transition percentage (%) for DPT system in ACN, DCM and CYH solvents.

| | Transition | λ | f | composition | CI(%) |
|-----|------------|-----------|--------|-------------|--------|
| | S0←S1 | 527 | 0.6040 | H←L | 99.90% |
| ACN | S0←S2 | 429 | 0.0000 | H-1←L | 99.30% |
| | S0←S3 | 368 | 0.0000 | H-2←L | 88.00% |
| | S0←S1 | 531 | 0.6141 | H←L | 99.90% |
| DCM | S0←S2 | 429 | 0.0000 | H-1←L | 99.30% |
| | S0←S3 | 368 | 0.0000 | H-2←L | 88.50% |
| | S0←S1 | 527 | 0.5939 | H←L | 99.80% |
| CYH | S0←S2 | 436 | 0.0000 | H-1←L | 99.30% |
| | S0←S3 | 357 | 0.0000 | H-3←L | 98.30% |

Table S6. Changes of dipole moment (D) for BP(OH)₂DCEt₂ molecule in CYH, DCM and ACN solvents of different states.

| | CYH | DCM | ACN |
|---------|---------|---------|---------|
| N | 0.00090 | 0.00052 | 0.00151 |
| N* | 0.00028 | 0.00030 | 0.00059 |
| T1*/T2* | 3.71037 | 4.39922 | 4.59632 |
| T3* | 0.00119 | 0.00136 | 0.00399 |

N represents enol form in S0 state;

T1 and T2 represent SPT form;

T3 represents DPT form;

The symbol "*" represents the form in S1 state

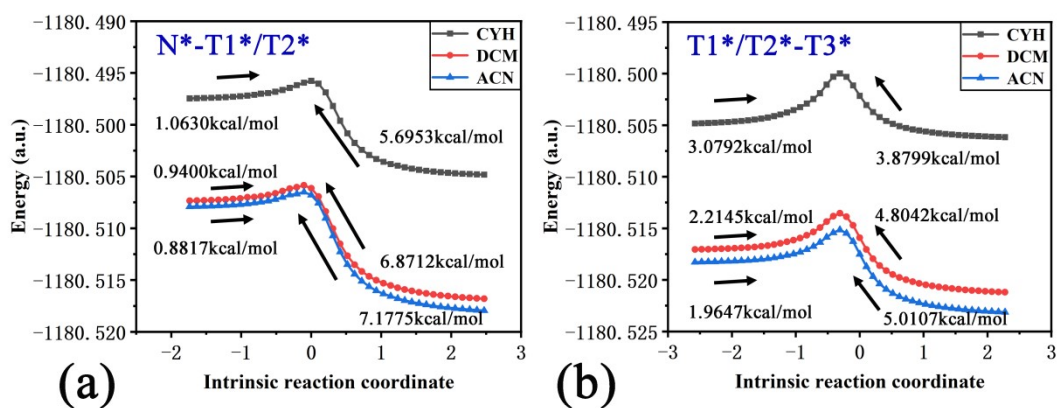


Figure S3. Comparison of S1 state Intrinsic reaction coordinates in different solvents. (a) The first step N*- T1* or N*-T2* in stepwise reaction path; (b)The second step T1*-T3* or T2*-T3* in stepwise reaction path.

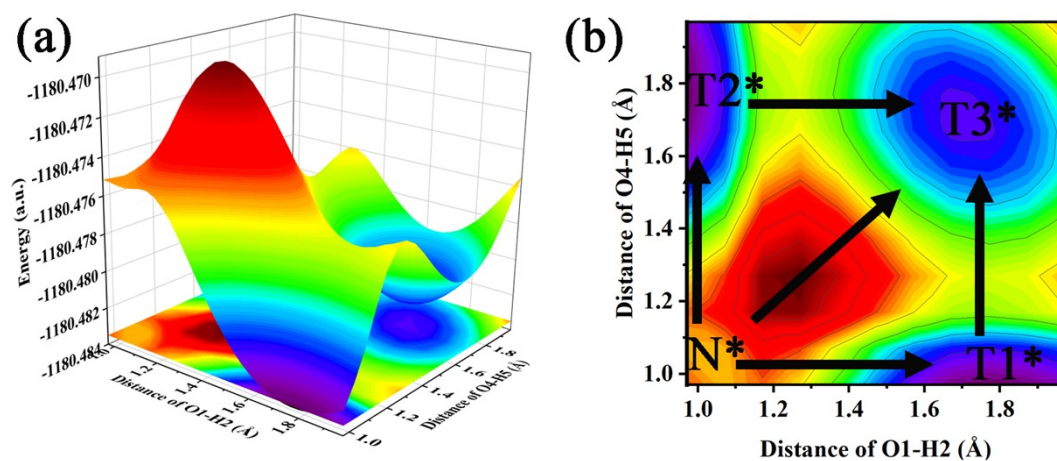


Figure S4. (a) S1 state PESs and (b) the S1 state projective plane for BP(OH)₂DCEt₂ in the the gas phase.

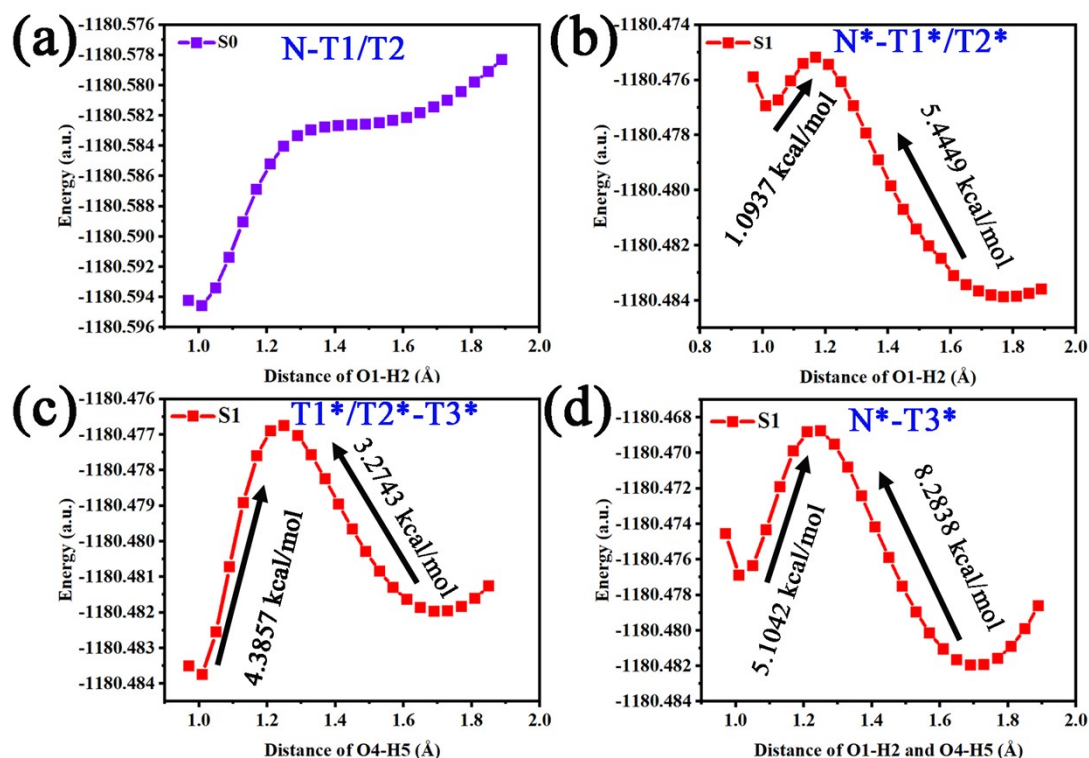


Figure S5. The potential energy curves of the gas phase. (a) The S0 state N-T1/T2 path; (b) The S1 state N*-T1*/T2* path; (c) The S1-state T1*/T2*-T3* path; (d) The S1-state N*-T3* path.

In Figure S4, the PESs of S1 state is symmetrical along with diagonal line. The PECs in S0 and S1 states in Figure S5 (a-d) indicate that the stepwise ESDPT process of BP(OH)₂DCET₂ occurs in S1 state.

Table S7. The Bond distances (Å) and bond angles (°) of double hydrogen bonds (O1-H2···N3 and O4-H5···N6) of BP(OH)₂DCET₂ under the application of the external electric field.

| | $E_x=0$ | | $E_x=10^{-4}$ | | $E_x=5 \times 10^{-4}$ | |
|---|---------|--------|---------------|--------|------------------------|--------|
| | S0 | S1 | S0 | S1 | S0 | S1 |
| O1-H2 | 0.9972 | 1.0195 | 0.9970 | 1.0200 | 0.9965 | 1.0217 |
| H2···N3 | 1.6967 | 1.6225 | 1.6976 | 1.6205 | 1.6998 | 1.6141 |
| $\delta(\text{O1-H2} \cdots \text{N3})$ | 148.07 | 150.33 | 148.05 | 150.40 | 148.00 | 150.60 |
| O4-H5 | 0.9972 | 1.0195 | 0.9974 | 1.0192 | 0.9980 | 1.0176 |
| H5···N6 | 1.6967 | 1.6225 | 1.6961 | 1.6240 | 1.6940 | 1.6305 |

| | | | | | | |
|---------------------------------------|---------------|--------|-----------------------|--------|-----------------------|--------|
| $\delta(\text{O4-H5}\cdots\text{N6})$ | 148.07 | 150.33 | 148.08 | 150.28 | 148.12 | 150.10 |
| | $E_x=10^{-3}$ | | $E_x=2\times 10^{-3}$ | | $E_x=3\times 10^{-3}$ | |
| | S0 | S1 | S0 | S1 | S0 | S1 |
| O1-H2 | 0.9957 | 1.0237 | 0.9943 | 1.0289 | 0.9930 | 1.0333 |
| H2 \cdots N3 | 1.7026 | 1.6066 | 1.7079 | 1.5895 | 1.7127 | 1.5755 |
| $\delta(\text{O1-H2}\cdots\text{N3})$ | 147.95 | 150.83 | 147.85 | 151.36 | 147.76 | 151.83 |
| O4-H5 | 0.9988 | 1.0155 | 1.0005 | 1.0104 | 1.0022 | 1.0049 |
| H5 \cdots N6 | 1.6910 | 1.6399 | 1.6850 | 1.6622 | 1.6783 | 1.6872 |
| $\delta(\text{O4-H5}\cdots\text{N6})$ | 148.18 | 149.82 | 148.30 | 149.20 | 148.45 | 148.54 |

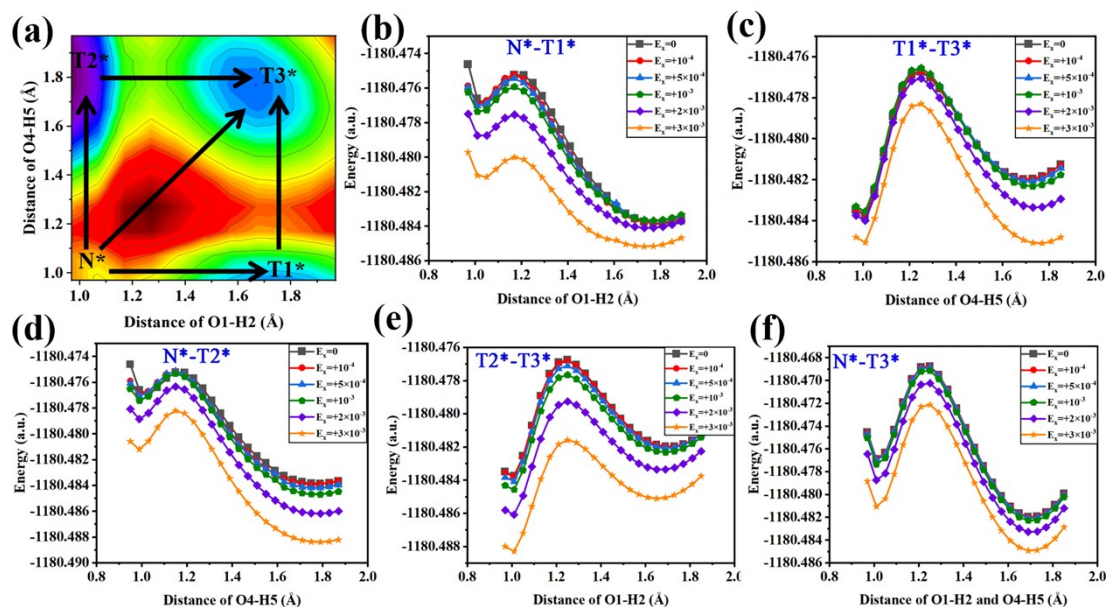


Figure S6. The potential energy curves of ESDPT path under the different external electric field. (a) The projective plane of the S1 state potential energy surface under $E_x = +3\times 10^{-3}$ a.u.; (b) The S1 state N*- T1* path; (c) The S1 state T1*-T3* path; (d) The S1 state N*-T2* path; (e) The S1 state T2*-T3* path; (f) The S1 state N*-T3* path.

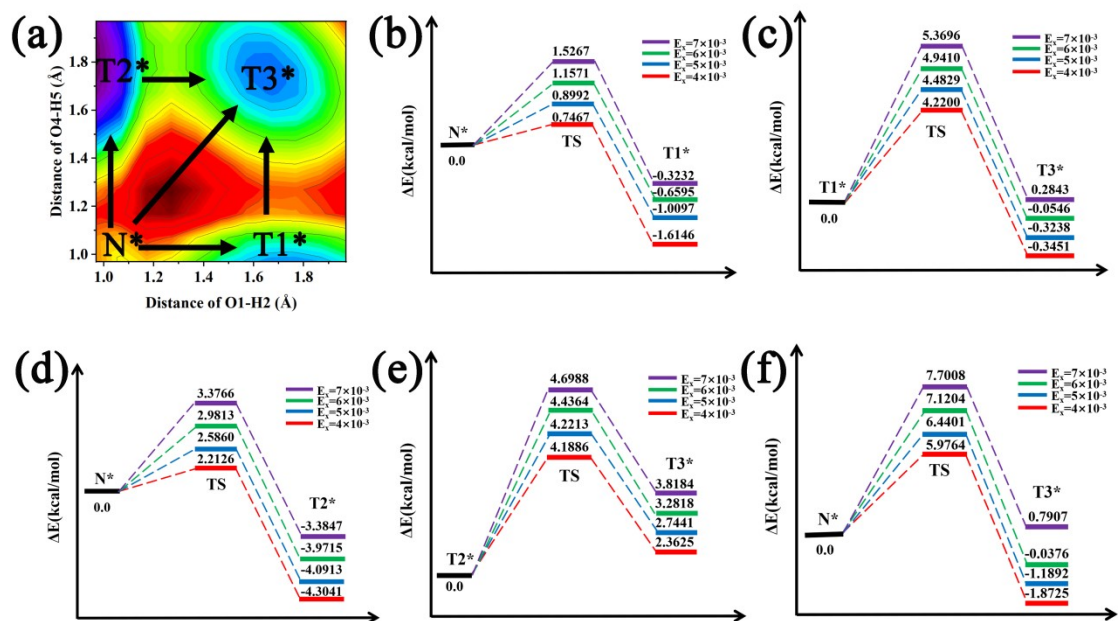


Figure S7. (a) The S1 state projective plane with $E_x = +3 \times 10^{-3}$ a.u. Calculated energy barriers for (b) N*-T1* path, (c) T1*-T3* path, (d) N*-T2* path, (e) T2*-T3* path and (f) N*-T3* path from $E_x = +4 \times 10^{-3}$ a.u. to $E_x = +7 \times 10^{-3}$ a.u. TS stands for transition-state structure energy.

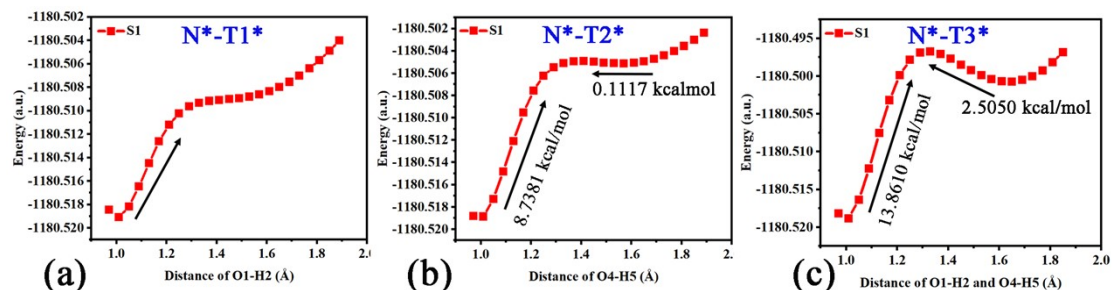


Figure S8. The potential energy curves with $E_x = +8 \times 10^{-3}$ a.u. (a) The S1 state N*-T1* path; (b) The S1 state N*-T2* path; (c) The S1 state N*-T3* path.

As shown in Figure S7, the results indicate that the forward energy barriers increase with the increasing EEF. The ESDPT process is difficult to occur due to the excessively large strength of the EEF. It is worth noting in Figure S8 that there is no stable keto structure existing when the EEF is applied to $E_x = +8 \times 10^{-3}$ a.u. Therefore, we only focus on the range of the EEF from $+1 \times 10^{-4}$ a.u. to $+3 \times 10^{-3}$ a.u. In addition, since the application of an external electric field less than $E_x = 10^{-4}$ has no effect on the energy barriers of ESDPT, we do not present the data.

Table S8. The potential barriers (kcal/mol) of path: N*-T1*-T3*, path: N*-T2*-T3* and path: N*-T3* under $E_x = 0$ a.u., $E_x = +3 \times 10^{-3}$ a.u., $E_y = +3 \times 10^{-3}$ a.u., $E_z = +3 \times 10^{-3}$ a.u. of S1 state potential energy curves.

| | | $E_x=0$ | $E_x=3 \times 10^{-3}$ | $E_y=3 \times 10^{-3}$ | $E_z=3 \times 10^{-3}$ |
|-----------------------|---------|---------|------------------------|------------------------|------------------------|
| Forward (kcal/mol) | N*-T1* | 1.0937 | 0.7210 | 0.9099 | 1.0768 |
| | T1*-T3* | 4.3856 | 4.2426 | 4.9573 | 4.9623 |
| | N*-T2* | 1.0937 | 1.8750 | 1.3228 | 1.0768 |
| | T2*-T3* | 4.3856 | 4.2068 | 4.1974 | 4.9623 |
| | N*-T3* | 5.1042 | 5.6011 | 5.1255 | 5.0803 |
| Reverse (kcal/mol) | T1*-N* | 5.4449 | 3.2461 | 5.7436 | 6.1829 |
| | T3*-T1* | 3.2743 | 4.2696 | 3.3333 | 3.3133 |
| | T2*-N* | 5.4449 | 6.3868 | 5.4775 | 6.1829 |
| | T3*-T2* | 3.2743 | 2.2075 | 3.2423 | 3.3133 |
| | T3*-N* | 8.2662 | 8.0327 | 8.2706 | 8.4312 |

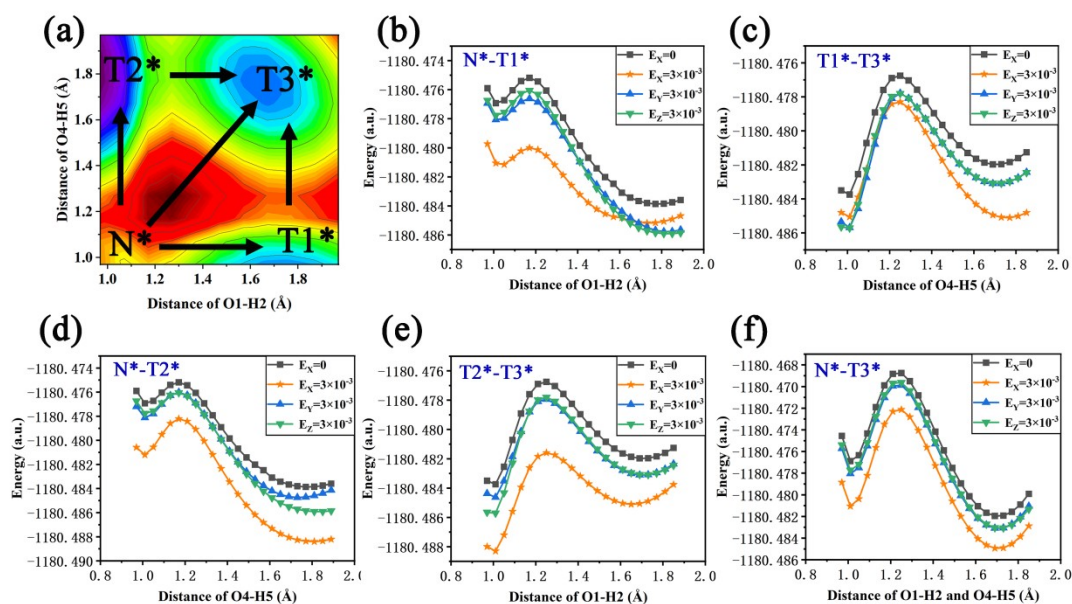


Figure S9. (a) The S1 state projective plane with $E_x = +3 \times 10^{-3}$ a.u. Calculated energy barriers for (b) N*-T1* path, (c) T1*-T3* path, (d) N*-T2* path, (e) T2*-T3* path and (f) N*-T3* path under $E_x = +3 \times 10^{-3}$ a.u., $E_y = +3 \times 10^{-3}$ a.u. and $E_z = +3 \times 10^{-3}$ a.u.

Cartesian coordinates of all structures

N represents the enol structure of BP(OH)₂DCEt₂ in S₀ state, T1 and T2 represent the form of the single proton transfer (SPT) along hydrogen bonds O1-H2...N3 or O4-H5...N6, T3 represents the form of the double proton transfer (DPT). N*, T1*/T2* and T3* represent the structure in S₁ state. TS* represents transition state structure in S₁ state.

The geometric structure coordinates of N in cyclohexane.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.71924400 | 0.15312400 | -0.00017200 |
| C | 2.88079900 | -0.71438300 | -0.00002700 |
| C | 3.44376900 | 0.56721000 | 0.00002400 |
| C | 2.59745900 | 1.66913800 | -0.00002100 |
| C | 1.21361000 | 1.48743000 | -0.00011400 |
| C | -0.71924400 | -0.15312800 | -0.00021500 |
| C | -1.21361100 | -1.48743300 | -0.00018200 |
| C | -2.59746100 | -1.66913900 | -0.00008100 |
| C | -3.44377000 | -0.56721100 | -0.00010600 |
| C | -2.88079800 | 0.71438200 | -0.00019600 |
| H | 3.50358900 | -1.59893000 | 0.00002300 |
| H | 3.00274700 | 2.67312500 | 0.00003700 |
| H | -3.00274900 | -2.67312700 | 0.00002600 |
| H | -3.50358800 | 1.59892900 | -0.00022700 |
| O | -0.42192500 | -2.56260600 | -0.00026200 |
| H | 0.51718200 | -2.22265100 | -0.00039000 |
| O | 0.42192100 | 2.56260200 | -0.00016900 |
| H | -0.51718500 | 2.22264400 | -0.00020000 |
| N | 1.56710100 | -0.89790500 | -0.00012600 |
| N | -1.56710000 | 0.89790300 | -0.00022900 |
| C | -4.91831200 | -0.79716300 | 0.00011700 |
| C | 4.91830900 | 0.79716600 | 0.00017800 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.43081000 | 1.89235800 | 0.00021700 |
| O | -5.43081800 | -1.89235400 | 0.00098600 |
| C | -7.05706900 | 0.24196200 | -0.00029600 |
| C | -7.61444600 | 1.64761300 | 0.00070700 |
| H | -7.36154900 | -0.32415900 | 0.88324400 |
| H | -7.36222000 | -0.32312900 | -0.88429400 |
| H | -7.28825400 | 2.19613800 | -0.88606200 |
| H | -8.70707700 | 1.61062900 | 0.00061400 |
| H | -7.28834200 | 2.19490600 | 0.88827500 |
| C | 7.05707100 | -0.24195900 | 0.00030300 |
| C | 7.61445700 | -1.64760900 | -0.00009400 |
| H | 7.36174400 | 0.32330400 | 0.88434000 |
| H | 7.36202900 | 0.32399200 | -0.88319800 |
| H | 7.28807600 | -2.19530600 | -0.88730200 |
| H | 8.70708800 | -1.61061900 | -0.00037800 |
| H | 7.28854400 | -2.19572800 | 0.88703500 |
| O | 5.60800400 | -0.35466700 | 0.00022100 |
| O | -5.60800400 | 0.35466900 | -0.00074400 |

The geometric structure coordinates of N* in cyclohexane.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.69568400 | -0.14305800 | -0.00007200 |
| C | -2.87308700 | 0.70378000 | -0.00031900 |
| C | -3.45011200 | -0.59061800 | -0.00018600 |
| C | -2.59452200 | -1.69964100 | 0.00004800 |
| C | -1.21433500 | -1.50116700 | 0.00012200 |
| C | 0.69570500 | 0.14287100 | -0.00005900 |
| C | 1.21427200 | 1.50100400 | -0.00019300 |
| C | 2.59444400 | 1.69957000 | -0.00011400 |
| C | 3.45010500 | 0.59060000 | 0.00005200 |
| C | 2.87316000 | -0.70383400 | 0.00012900 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.51063900 | 1.57902500 | -0.00048800 |
| H | -2.99227300 | -2.70586200 | 0.00018200 |
| H | 2.99213000 | 2.70581700 | -0.00019800 |
| H | 3.51076700 | -1.57903900 | 0.00025200 |
| O | 0.39904700 | 2.54140100 | -0.00041100 |
| H | -0.55207600 | 2.16945000 | -0.00053600 |
| O | -0.39920000 | -2.54163200 | 0.00039700 |
| H | 0.55195900 | -2.16975700 | 0.00052200 |
| N | -1.57091300 | 0.91566800 | -0.00026800 |
| N | 1.57099900 | -0.91580300 | 0.00008600 |
| C | 4.90787400 | 0.80403300 | 0.00013700 |
| C | -4.90789500 | -0.80395900 | -0.00026600 |
| O | -5.43741800 | -1.89757900 | 0.00012100 |
| O | 5.43732800 | 1.89768500 | -0.00001900 |
| C | 7.04195100 | -0.24962600 | 0.00008100 |
| C | 7.59995800 | -1.65573800 | 0.00032300 |
| H | 7.35155500 | 0.31577500 | 0.88305300 |
| H | 7.35155800 | 0.31545600 | -0.88309800 |
| H | 7.27311200 | -2.20389300 | -0.88663000 |
| H | 8.69274300 | -1.62033800 | 0.00030000 |
| H | 7.27313700 | -2.20358300 | 0.88747700 |
| C | -7.04190700 | 0.24983200 | 0.00010200 |
| C | -7.59982700 | 1.65597900 | 0.00012700 |
| H | -7.35139000 | -0.31534200 | 0.88326400 |
| H | -7.35170400 | -0.31543800 | -0.88288800 |
| H | -7.27311700 | 2.20391200 | -0.88701300 |
| H | -8.69261400 | 1.62064600 | 0.00032300 |
| H | -7.27280200 | 2.20400600 | 0.88709400 |
| O | -5.59735800 | 0.36055200 | -0.00016100 |
| O | 5.59740900 | -0.36043500 | 0.00009600 |

The geometric structure coordinates of T1*/T2* in cyclohexane.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.68771400 | 0.15262400 | -0.00000800 |
| C | 2.92661100 | -0.71225700 | -0.00009400 |
| C | 3.46616600 | 0.57273200 | 0.00002900 |
| C | 2.58982900 | 1.67618000 | 0.00013800 |
| C | 1.20648400 | 1.47994100 | 0.00011900 |
| C | -0.72920900 | -0.16853800 | -0.00003600 |
| C | -1.22164900 | -1.55633500 | -0.00018200 |
| C | -2.63016300 | -1.71503800 | -0.00019200 |
| C | -3.47683200 | -0.59890900 | -0.00006300 |
| C | -2.90308500 | 0.67678600 | 0.00007700 |
| H | 3.53639800 | -1.60354800 | -0.00017500 |
| H | 2.98392800 | 2.68342900 | 0.00023300 |
| H | -3.03895600 | -2.71719800 | -0.00030300 |
| H | -3.52049700 | 1.56491000 | 0.00017500 |
| O | -0.41281100 | -2.53808400 | -0.00030300 |
| H | 1.15250700 | -1.81547000 | -0.00019700 |
| O | 0.40317600 | 2.53753200 | 0.00021100 |
| H | -0.53922400 | 2.18357700 | 0.00016400 |
| N | 1.60795900 | -0.87922100 | -0.00010500 |
| N | -1.57180800 | 0.87556800 | 0.00009000 |
| C | -4.94453300 | -0.80090900 | -0.00007700 |
| C | 4.92624100 | 0.80173900 | 0.00004600 |
| O | 5.43802700 | 1.90123100 | 0.00019700 |
| O | -5.47997900 | -1.88844900 | -0.00019300 |
| C | -7.07064700 | 0.26715200 | 0.00009100 |
| C | -7.61599300 | 1.67817600 | 0.00025800 |
| H | -7.38441400 | -0.29520200 | 0.88328500 |
| H | -7.38444200 | -0.29500200 | -0.88322100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.28431100 | 2.22332800 | -0.88672400 |
| H | -8.70905200 | 1.65237600 | 0.00027300 |
| H | -7.28428200 | 2.22313000 | 0.88735200 |
| C | 7.07048000 | -0.23244300 | -0.00000900 |
| C | 7.63826100 | -1.63429600 | -0.00009700 |
| H | 7.37393900 | 0.33479500 | 0.88355000 |
| H | 7.37397800 | 0.33492300 | -0.88347200 |
| H | 7.31627500 | -2.18459700 | -0.88746100 |
| H | 8.73063400 | -1.59021600 | -0.00007200 |
| H | 7.31624000 | -2.18472100 | 0.88717700 |
| O | 5.62454900 | -0.35425600 | -0.00005000 |
| O | -5.62418900 | 0.36595400 | 0.00007900 |

The geometric structure coordinates of T3* in cyclohexane.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.68461200 | 0.16878900 | 0.00004900 |
| C | 2.92953800 | -0.69123900 | 0.00003900 |
| C | 3.47185500 | 0.59575800 | 0.00015000 |
| C | 2.61230400 | 1.70006700 | 0.00021200 |
| C | 1.19672700 | 1.54728000 | 0.00016600 |
| C | -0.68458500 | -0.16907100 | -0.00001300 |
| C | -1.19682500 | -1.54752400 | -0.00010800 |
| C | -2.61242100 | -1.70016900 | -0.00014700 |
| C | -3.47186900 | -0.59578200 | -0.00010300 |
| C | -2.92943400 | 0.69116600 | -0.00001900 |
| H | 3.53677000 | -1.58391200 | -0.00000700 |
| H | 3.01641800 | 2.70388200 | 0.00030200 |
| H | -3.01663200 | -2.70394500 | -0.00021400 |
| H | -3.53658200 | 1.58389500 | 0.00000600 |
| O | -0.40292100 | -2.53224000 | -0.00015400 |
| H | 1.15817400 | -1.80049800 | -0.00008700 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.40270100 | 2.53190200 | 0.00023600 |
| H | -1.15794700 | 1.80025500 | 0.00008400 |
| N | 1.60434200 | -0.86123900 | -0.00000400 |
| N | -1.60422300 | 0.86103800 | 0.00001700 |
| C | -4.93877400 | -0.80775200 | -0.00014600 |
| C | 4.93873900 | 0.80786100 | 0.00020700 |
| O | 5.46582100 | 1.89824900 | 0.00021300 |
| O | -5.46595600 | -1.89809000 | -0.00016900 |
| C | -7.07009400 | 0.25326800 | -0.00001700 |
| C | -7.61974100 | 1.66238600 | 0.00015500 |
| H | -7.38079800 | -0.31019500 | 0.88339800 |
| H | -7.38085300 | -0.30999800 | -0.88354000 |
| H | -7.29054100 | 2.20864000 | -0.88707700 |
| H | -8.71262900 | 1.63256200 | 0.00018600 |
| H | -7.29048600 | 2.20844500 | 0.88748800 |
| C | 7.07015200 | -0.25297400 | -0.00008200 |
| C | 7.61992000 | -1.66204400 | -0.00033300 |
| H | 7.38088900 | 0.31028100 | 0.88345500 |
| H | 7.38078000 | 0.31055300 | -0.88348400 |
| H | 7.29068900 | -2.20809300 | -0.88768000 |
| H | 8.71280600 | -1.63212400 | -0.00039200 |
| H | 7.29079300 | -2.20836600 | 0.88688500 |
| O | 5.62282800 | -0.35642300 | -0.00000500 |
| O | -5.62276200 | 0.35659100 | -0.00005400 |

The geometric structure coordinates of TS* of N*-T1*/T2* path in cyclohexane.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.68335592 | 0.22215766 | 0.00000731 |
| C | -2.85192892 | -0.69488434 | -0.00015769 |
| C | -3.44440392 | 0.58633466 | 0.00006131 |
| C | -2.60712692 | 1.71677766 | 0.00025731 |

| | | | |
|---|-------------|-------------|-------------|
| C | -1.22375692 | 1.55319766 | 0.00023031 |
| C | 0.70994708 | -0.07023634 | -0.00002169 |
| C | 1.18264308 | -1.45659434 | -0.00023369 |
| C | 2.56532208 | -1.68531134 | -0.00025969 |
| C | 3.44162008 | -0.59344534 | -0.00007269 |
| C | 2.89769908 | 0.71127966 | 0.00013231 |
| H | -3.46085892 | -1.58906634 | -0.00030969 |
| H | -3.03133692 | 2.71207666 | 0.00042431 |
| H | 2.94133308 | -2.69990534 | -0.00041569 |
| H | 3.55610608 | 1.57060066 | 0.00027931 |
| O | 0.31729508 | -2.42930634 | -0.00038769 |
| H | -0.72715292 | -1.90458934 | -0.00032969 |
| O | -0.42834092 | 2.61718266 | 0.00041231 |
| H | 0.51804908 | 2.28037766 | 0.00036031 |
| N | -1.54355992 | -0.85704934 | -0.00017969 |
| N | 1.59180908 | 0.96320166 | 0.00015431 |
| C | 4.89791408 | -0.83696934 | -0.00009069 |
| C | -4.90524292 | 0.77271566 | 0.00009231 |
| O | -5.45519992 | 1.85629966 | 0.00031631 |
| O | 5.40231908 | -1.94115134 | -0.00028769 |
| C | 7.05379708 | 0.17080666 | 0.00015431 |
| C | 7.64060008 | 1.56503066 | 0.00038831 |
| H | 7.35097508 | -0.40048334 | -0.88314669 |
| H | 7.35093108 | -0.40076034 | 0.88329231 |
| H | 7.32546908 | 2.11957966 | 0.88756331 |
| H | 8.73235908 | 1.50666866 | 0.00041431 |
| H | 7.32552708 | 2.11985166 | -0.88663769 |
| C | -7.01976692 | -0.32036834 | -0.00013669 |
| C | -7.55211892 | -1.73645234 | -0.00037669 |
| H | -7.33992992 | 0.23909866 | -0.88309769 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.33992092 | 0.23879666 | 0.88301931 |
| H | -7.21541192 | -2.27860634 | 0.88660231 |
| H | -8.64538392 | -1.72097834 | -0.00037269 |
| H | -7.21541292 | -2.27830834 | -0.88753769 |
| O | -5.57358992 | -0.40483034 | -0.00015969 |
| O | 5.61097308 | 0.31146666 | 0.00014131 |

The geometric structure coordinates of TS* of T1*/T2*-T3* path in cyclohexane.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.69178829 | -0.06145966 | 0.00001432 |
| C | -2.95180529 | 0.72917834 | -0.00006768 |
| C | -3.44593329 | -0.57728566 | 0.00007432 |
| C | -2.54626029 | -1.65631566 | 0.00018832 |
| C | -1.15660029 | -1.43155666 | 0.00016032 |
| C | 0.69301871 | 0.25866734 | -0.00002268 |
| C | 1.22573671 | 1.62572334 | -0.00017668 |
| C | 2.64139771 | 1.74123134 | -0.00019668 |
| C | 3.45969671 | 0.60240934 | -0.00007368 |
| C | 2.86420871 | -0.66630366 | 0.00007032 |
| H | -3.59368029 | 1.59726634 | -0.00015868 |
| H | -2.91646829 | -2.67281166 | 0.00029732 |
| H | 3.08101971 | 2.73015034 | -0.00030768 |
| H | 3.45387771 | -1.57213766 | 0.00016732 |
| O | 0.43635571 | 2.61766434 | -0.00028368 |
| H | -1.22291729 | 1.89250534 | -0.00019168 |
| O | -0.29561429 | -2.40083166 | 0.00025732 |
| H | 0.78851571 | -1.83062066 | 0.00019832 |
| N | -1.63710729 | 0.94515734 | -0.00009068 |
| N | 1.53477071 | -0.81328166 | 0.00009032 |
| C | 4.93100771 | 0.76582734 | -0.00009968 |
| C | -4.90254629 | -0.84558466 | 0.00010132 |

| | | | |
|---|-------------|-------------|-------------|
| O | -5.38504029 | -1.95705266 | 0.00023332 |
| O | 5.49513671 | 1.83886434 | -0.00025168 |
| C | 7.02862771 | -0.35849866 | 0.00004532 |
| C | 7.53769571 | -1.78298166 | 0.00021332 |
| H | 7.35677971 | 0.19561234 | 0.88321932 |
| H | 7.35676371 | 0.19539834 | -0.88326968 |
| H | 7.19251571 | -2.31959966 | -0.88683868 |
| H | 8.63106471 | -1.78475566 | 0.00020632 |
| H | 7.19252671 | -2.31938866 | 0.88739632 |
| C | -7.07414529 | 0.12918834 | -0.00003568 |
| C | -7.68083629 | 1.51457334 | -0.00017968 |
| H | -7.36145729 | -0.44627166 | 0.88356032 |
| H | -7.36144229 | -0.44644866 | -0.88352168 |
| H | -7.37474329 | 2.07373334 | -0.88759668 |
| H | -8.77148929 | 1.43953134 | -0.00018568 |
| H | -7.37476529 | 2.07390734 | 0.88713632 |
| O | -5.63167529 | 0.29064034 | -0.00003968 |
| O | 5.58005471 | -0.41961566 | 0.00006632 |

The geometric structure coordinates of N in dichloromethane.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.71916700 | 0.15295000 | 0.00013300 |
| C | 2.88143100 | -0.71509700 | 0.00036400 |
| C | 3.44380100 | 0.56686800 | 0.00030000 |
| C | 2.59692100 | 1.66870700 | 0.00014600 |
| C | 1.21383900 | 1.48599800 | 0.00007300 |
| C | -0.71916100 | -0.15300100 | 0.00001300 |
| C | -1.21385500 | -1.48604300 | 0.00007600 |
| C | -2.59694100 | -1.66872600 | 0.00000500 |
| C | -3.44380200 | -0.56687300 | -0.00016500 |
| C | -2.88141100 | 0.71508200 | -0.00025300 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.50216600 | -1.60128900 | 0.00049000 |
| H | 3.00045300 | 2.67360100 | 0.00010000 |
| H | -3.00049100 | -2.67361300 | 0.00008200 |
| H | -3.50213100 | 1.60128600 | -0.00038100 |
| O | -0.41988400 | -2.56303100 | 0.00013500 |
| H | 0.51995900 | -2.22146800 | 0.00004400 |
| O | 0.41984300 | 2.56296900 | -0.00008000 |
| H | -0.51999200 | 2.22138700 | 0.00001900 |
| N | 1.56707500 | -0.89812400 | 0.00028700 |
| N | -1.56705200 | 0.89808600 | -0.00016700 |
| C | -4.91854700 | -0.79662400 | -0.00014900 |
| C | 4.91854200 | 0.79664400 | 0.00043500 |
| O | 5.42814900 | 1.89587700 | -0.00004700 |
| O | -5.42817200 | -1.89584800 | 0.00043700 |
| C | -7.06153600 | 0.24251400 | -0.00034900 |
| C | -7.61268000 | 1.65001800 | 0.00041700 |
| H | -7.36617400 | -0.31987500 | 0.88520800 |
| H | -7.36667400 | -0.31908200 | -0.88625100 |
| H | -7.28575500 | 2.19659600 | -0.88763900 |
| H | -8.70536500 | 1.61322100 | 0.00042900 |
| H | -7.28569000 | 2.19567800 | 0.88901300 |
| C | 7.06154700 | -0.24245800 | -0.00030500 |
| C | 7.61271300 | -1.64995200 | -0.00056400 |
| H | 7.36670000 | 0.31948800 | 0.88536500 |
| H | 7.36615000 | 0.31959300 | -0.88609400 |
| H | 7.28529100 | -2.19607400 | -0.88871800 |
| H | 8.70539700 | -1.61313000 | -0.00115100 |
| H | 7.28624200 | -2.19608100 | 0.88793500 |
| O | 5.60859900 | -0.35018700 | 0.00022000 |
| O | -5.60858600 | 0.35021900 | -0.00070900 |

The geometric structure coordinates of N* in dichloromethane.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69252600 | -0.14199400 | 0.00006200 |
| C | 2.87114000 | 0.70498400 | 0.00017000 |
| C | 3.44783800 | -0.59188600 | 0.00001900 |
| C | 2.59183100 | -1.70104300 | -0.00006300 |
| C | 1.21233000 | -1.50236400 | -0.00001400 |
| C | -0.69254500 | 0.14182800 | 0.00002400 |
| C | -1.21227400 | 1.50221900 | 0.00008500 |
| C | -2.59176200 | 1.70098000 | 0.00011700 |
| C | -3.44783100 | 0.59187000 | 0.00003600 |
| C | -2.87120500 | -0.70503100 | -0.00008200 |
| H | 3.50790200 | 1.58103900 | 0.00025200 |
| H | 2.98636500 | -2.70889500 | -0.00013500 |
| H | -2.98623800 | 2.70885500 | 0.00017100 |
| H | -3.50801500 | -1.58105200 | -0.00015100 |
| O | -0.39583200 | 2.54144900 | 0.00004700 |
| H | 0.55667700 | 2.16828800 | -0.00021900 |
| O | 0.39596700 | -2.54165200 | 0.00002400 |
| H | -0.55657300 | -2.16855500 | 0.00027100 |
| N | 1.57094900 | 0.91783700 | 0.00018400 |
| N | -1.57102500 | -0.91795600 | -0.00008100 |
| C | -4.90475600 | 0.80377300 | 0.00003800 |
| C | 4.90477500 | -0.80370800 | -0.00002900 |
| O | 5.43383500 | -1.90086200 | -0.00014000 |
| O | -5.43375500 | 1.90095700 | 0.00007800 |
| C | -7.04326100 | -0.25013800 | -0.00015900 |
| C | -7.59520600 | -1.65814100 | -0.00041200 |
| H | -7.35356200 | 0.31157400 | -0.88498800 |
| H | -7.35368900 | 0.31130200 | 0.88479900 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.26748400 | -2.20454800 | 0.88762200 |
| H | -8.68803000 | -1.62316900 | -0.00047500 |
| H | -7.26737000 | -2.20427300 | -0.88857300 |
| C | 7.04322200 | 0.25032100 | 0.00004500 |
| C | 7.59509100 | 1.65835400 | 0.00016700 |
| H | 7.35360500 | -0.31115700 | -0.88490400 |
| H | 7.35363100 | -0.31131900 | 0.88488200 |
| H | 7.26729500 | 2.20452400 | 0.88831900 |
| H | 8.68791600 | 1.62344300 | 0.00014700 |
| H | 7.26726800 | 2.20468700 | -0.88787600 |
| O | 5.59539000 | 0.35609200 | 0.00007600 |
| O | -5.59543400 | -0.35598900 | -0.00007000 |

The geometric structure coordinates of T1*/T2* in dichloromethane.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.68191700 | 0.12533600 | -0.00004800 |
| C | 2.93366500 | -0.72104300 | -0.00015300 |
| C | 3.46525100 | 0.56766000 | -0.00006400 |
| C | 2.58053500 | 1.66477200 | 0.00003200 |
| C | 1.20082900 | 1.46014000 | 0.00003700 |
| C | -0.72069800 | -0.18894200 | -0.00001700 |
| C | -1.22875800 | -1.57736500 | -0.00006900 |
| C | -2.64254100 | -1.72544900 | -0.00004100 |
| C | -3.48009700 | -0.60640500 | 0.00004100 |
| C | -2.89281800 | 0.67078800 | 0.00009800 |
| H | 3.54506200 | -1.61153600 | -0.00023200 |
| H | 2.96471700 | 2.67624400 | 0.00009500 |
| H | -3.05393200 | -2.72704500 | -0.00007500 |
| H | -3.50644900 | 1.56219500 | 0.00017200 |
| O | -0.43454600 | -2.56427600 | -0.00013500 |
| H | 1.19424100 | -1.84207400 | -0.00018700 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.39142300 | 2.51322900 | 0.00011300 |
| H | -0.55322200 | 2.15055000 | 0.00009100 |
| N | 1.61637300 | -0.89943200 | -0.00014800 |
| N | -1.56899400 | 0.86343200 | 0.00006800 |
| C | -4.94734600 | -0.79286400 | 0.00007400 |
| C | 4.92279200 | 0.80780400 | -0.00007600 |
| O | 5.42299000 | 1.91572600 | 0.00004300 |
| O | -5.49362100 | -1.87898700 | 0.00004400 |
| C | -7.06791000 | 0.29566800 | 0.00017700 |
| C | -7.59497300 | 1.71316300 | 0.00024700 |
| H | -7.38750800 | -0.26019000 | 0.88517400 |
| H | -7.38756400 | -0.26012300 | -0.88484100 |
| H | -7.25775900 | 2.25365800 | -0.88784700 |
| H | -8.68825600 | 1.69730300 | 0.00028000 |
| H | -7.25770400 | 2.25359100 | 0.88836000 |
| C | 7.08064800 | -0.20604900 | -0.00010500 |
| C | 7.65441300 | -1.60494500 | -0.00017200 |
| H | 7.37974200 | 0.36020600 | 0.88532600 |
| H | 7.37976800 | 0.36030100 | -0.88546700 |
| H | 7.33585300 | -2.15619100 | -0.88849500 |
| H | 8.74643700 | -1.55186100 | -0.00015300 |
| H | 7.33582700 | -2.15628600 | 0.88808300 |
| O | 5.63257200 | -0.33597200 | -0.00013500 |
| O | -5.61761400 | 0.37648600 | 0.00013400 |

The geometric structure coordinates of T3* in dichloromethane.

| | | | |
|---|------------|-------------|-------------|
| C | 0.68276800 | 0.16645000 | -0.00000300 |
| C | 2.93271400 | -0.69390300 | -0.00029200 |
| C | 3.47814100 | 0.59235600 | -0.00013700 |
| C | 2.61859300 | 1.69615600 | 0.00008000 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.20170300 | 1.54633900 | 0.00015200 |
| C | -0.68274200 | -0.16672700 | 0.00006400 |
| C | -1.20180000 | -1.54657800 | -0.00008000 |
| C | -2.61870700 | -1.69625700 | 0.00001200 |
| C | -3.47815500 | -0.59238200 | 0.00023300 |
| C | -2.93261300 | 0.69382900 | 0.00036200 |
| H | 3.53374400 | -1.59107500 | -0.00047300 |
| H | 3.02064100 | 2.70129500 | 0.00019500 |
| H | -3.02084900 | -2.70135800 | -0.00008500 |
| H | -3.53356400 | 1.59105400 | 0.00053900 |
| O | -0.41554100 | -2.53572400 | -0.00026400 |
| H | 1.18102500 | -1.80462500 | -0.00033500 |
| O | 0.41532300 | 2.53539000 | 0.00033900 |
| H | -1.18081900 | 1.80438700 | 0.00037800 |
| N | 1.60827800 | -0.86221800 | -0.00023100 |
| N | -1.60816400 | 0.86202000 | 0.00028700 |
| C | -4.94443700 | -0.80391500 | 0.00034000 |
| C | 4.94440300 | 0.80402100 | -0.00020800 |
| O | 5.46837200 | 1.89935000 | 0.00003700 |
| O | -5.46850500 | -1.89919700 | -0.00001100 |
| C | -7.08150300 | 0.25314200 | 0.00003300 |
| C | -7.62699300 | 1.66334400 | -0.00002700 |
| H | -7.39205700 | -0.30705600 | 0.88531800 |
| H | -7.39180300 | -0.30703200 | -0.88535500 |
| H | -7.29727100 | 2.20816300 | -0.88825200 |
| H | -8.71989400 | 1.63229900 | -0.00018600 |
| H | -7.29752900 | 2.20813900 | 0.88830800 |
| C | 7.08156100 | -0.25285000 | -0.00020700 |
| C | 7.62717300 | -1.66300400 | -0.00028100 |
| H | 7.39189900 | 0.30730100 | 0.88518300 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.39197900 | 0.30742600 | -0.88549000 |
| H | 7.29766700 | -2.20777900 | -0.88861400 |
| H | 8.72007100 | -1.63186400 | -0.00023100 |
| H | 7.29758800 | -2.20790200 | 0.88794600 |
| O | 5.63100700 | -0.35349400 | -0.00028300 |
| O | -5.63094100 | 0.35366000 | 0.00024800 |

The geometric structure coordinates of TS* of N*-T1*/T2* path in dichloromethane.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.67835141 | 0.21578615 | -0.00000859 |
| C | 2.84983041 | -0.69616885 | -0.00009659 |
| C | 3.44111741 | 0.58743315 | -0.00001159 |
| C | 2.60254841 | 1.71718715 | 0.00007541 |
| C | 1.22054241 | 1.55166815 | 0.00007841 |
| C | -0.70574159 | -0.07330285 | -0.00000759 |
| C | -1.18006159 | -1.46056685 | -0.00009559 |
| C | -2.56345459 | -1.68786285 | -0.00008659 |
| C | -3.43802759 | -0.59541085 | 0.00000441 |
| C | -2.89294359 | 0.71386415 | 0.00008541 |
| H | 3.45865341 | -1.59070285 | -0.00016559 |
| H | 3.02264941 | 2.71451715 | 0.00013941 |
| H | -2.93762059 | -2.70348485 | -0.00014959 |
| H | -3.55139859 | 1.57350215 | 0.00015541 |
| O | -0.31649759 | -2.43434585 | -0.00017759 |
| H | 0.72582241 | -1.91408285 | -0.00015759 |
| O | 0.42096841 | 2.61161115 | 0.00015941 |
| H | -0.52792259 | 2.26917315 | 0.00014941 |
| N | 1.54254941 | -0.86227485 | -0.00009459 |
| N | -1.59226359 | 0.96528215 | 0.00007941 |
| C | -4.89337459 | -0.83589185 | 0.00001741 |
| C | 4.90133441 | 0.77396415 | -0.00001359 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.44904741 | 1.86182715 | 0.00005741 |
| O | -5.39921859 | -1.94300485 | -0.00005259 |
| C | -7.05253159 | 0.17519315 | 0.00014441 |
| C | -7.63093059 | 1.57247915 | 0.00026541 |
| H | -7.35160659 | -0.39214985 | 0.88514241 |
| H | -7.35165359 | -0.39201585 | -0.88492259 |
| H | -7.31360159 | 2.12488915 | -0.88781059 |
| H | -8.72287059 | 1.51674815 | 0.00029041 |
| H | -7.31355459 | 2.12475515 | 0.88840841 |
| C | 7.02158541 | -0.31650085 | -0.00012259 |
| C | 7.54949041 | -1.73370285 | -0.00022259 |
| H | 7.34154341 | 0.23953815 | 0.88480641 |
| H | 7.34151441 | 0.23965115 | -0.88499059 |
| H | 7.21254741 | -2.27429585 | -0.88837559 |
| H | 8.64276041 | -1.71726985 | -0.00024059 |
| H | 7.21257841 | -2.27440985 | 0.88787341 |
| O | 5.57204041 | -0.39759985 | -0.00010459 |
| O | -5.60652859 | 0.30893815 | 0.00011741 |

The geometric structure coordinates of TS* of T1*/T2*-T3* path in dichloromethane.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.68892567 | -0.04678075 | 0.00001518 |
| C | -2.95680067 | 0.73381125 | -0.00009482 |
| C | -3.44801067 | -0.57383075 | 0.00001218 |
| C | -2.54302267 | -1.64958975 | 0.00012318 |
| C | -1.15676767 | -1.41830975 | 0.00012618 |
| C | 0.69010033 | 0.26932825 | 0.00000718 |
| C | 1.23109833 | 1.63834325 | -0.00010282 |
| C | 2.65027433 | 1.74653525 | -0.00010182 |
| C | 3.46360133 | 0.60644725 | -0.00000182 |
| C | 2.85951633 | -0.66212175 | 0.00010518 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.59663267 | 1.60382325 | -0.00018082 |
| H | -2.90606067 | -2.66897875 | 0.00020618 |
| H | 3.09043033 | 2.73570925 | -0.00018082 |
| H | 3.44512133 | -1.57102575 | 0.00018818 |
| O | 0.45279733 | 2.63466225 | -0.00019082 |
| H | -1.25379267 | 1.90802925 | -0.00016382 |
| O | -0.29460767 | -2.39118975 | 0.00022518 |
| H | 0.77348933 | -1.83350675 | 0.00018918 |
| N | -1.64341467 | 0.95558125 | -0.00008982 |
| N | 1.53381933 | -0.80574075 | 0.00010818 |
| C | 4.93468833 | 0.76021025 | -0.00000582 |
| C | -4.90243967 | -0.84835475 | 0.00000618 |
| O | -5.37675867 | -1.96673075 | 0.00009918 |
| O | 5.50480433 | 1.83374425 | -0.00009182 |
| C | 7.03004333 | -0.37729675 | 0.00011218 |
| C | 7.52398533 | -1.80662675 | 0.00022418 |
| H | 7.36223333 | 0.17103625 | 0.88513118 |
| H | 7.36225533 | 0.17090525 | -0.88498182 |
| H | 7.17446633 | -2.33919475 | -0.88790782 |
| H | 8.61733633 | -1.81592275 | 0.00024018 |
| H | 7.17444033 | -2.33906375 | 0.88842418 |
| C | -7.08354067 | 0.11480925 | -0.00014082 |
| C | -7.68920467 | 1.50014125 | -0.00031382 |
| H | -7.36924967 | -0.45815075 | 0.88535018 |
| H | -7.36919667 | -0.45834775 | -0.88552282 |
| H | -7.38340267 | 2.05849225 | -0.88867382 |
| H | -8.77969667 | 1.42193125 | -0.00033682 |
| H | -7.38345567 | 2.05869125 | 0.88793918 |
| O | -5.63858067 | 0.27801325 | -0.00011582 |
| O | 5.57800433 | -0.42429975 | 0.00009818 |

The geometric structure coordinates of N in acetonitrile.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.71905100 | 0.15298300 | 0.00002100 |
| C | 2.88141200 | -0.71501200 | -0.00003100 |
| C | 3.44352700 | 0.56697600 | 0.00002900 |
| C | 2.59645700 | 1.66870400 | 0.00009900 |
| C | 1.21351200 | 1.48595400 | 0.00009400 |
| C | -0.71904500 | -0.15304500 | -0.00001200 |
| C | -1.21353200 | -1.48600900 | -0.00002000 |
| C | -2.59648100 | -1.66872700 | 0.00003200 |
| C | -3.44352900 | -0.56698100 | 0.00000800 |
| C | -2.88138800 | 0.71499400 | -0.00003000 |
| H | 3.50168700 | -1.60143200 | -0.00009000 |
| H | 2.99975800 | 2.67365900 | 0.00015800 |
| H | -2.99980400 | -2.67367400 | 0.00007000 |
| H | -3.50164500 | 1.60142800 | -0.00004000 |
| O | -0.41863800 | -2.56278800 | -0.00008800 |
| H | 0.52084700 | -2.21909900 | -0.00024100 |
| O | 0.41858800 | 2.56271300 | 0.00016900 |
| H | -0.52088700 | 2.21900100 | 0.00025700 |
| N | 1.56692600 | -0.89802300 | -0.00002400 |
| N | -1.56689900 | 0.89797800 | -0.00002000 |
| C | -4.91849600 | -0.79654000 | 0.00012100 |
| C | 4.91849000 | 0.79656500 | 0.00003000 |
| O | 5.42750000 | 1.89651000 | 0.00020800 |
| O | -5.42752900 | -1.89647500 | 0.00091000 |
| C | -7.06206800 | 0.24267400 | -0.00034800 |
| C | -7.61346800 | 1.64980000 | -0.00001400 |
| H | -7.36676400 | -0.31864200 | 0.88573800 |
| H | -7.36720000 | -0.31834900 | -0.88648200 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.28741400 | 2.19616800 | -0.88853700 |
| H | -8.70606100 | 1.61112200 | 0.00002200 |
| H | -7.28733000 | 2.19578400 | 0.88871400 |
| C | 7.06208200 | -0.24260600 | 0.00002400 |
| C | 7.61351000 | -1.64972100 | -0.00032800 |
| H | 7.36696400 | 0.31834900 | 0.88628400 |
| H | 7.36700500 | 0.31879100 | -0.88593700 |
| H | 7.28729600 | -2.19571700 | -0.88902100 |
| H | 8.70610200 | -1.61101700 | -0.00048200 |
| H | 7.28755700 | -2.19608900 | 0.88823000 |
| O | 5.60822600 | -0.34969400 | -0.00002300 |
| O | -5.60821000 | 0.34973200 | -0.00072400 |

The geometric structure coordinates of N* in acetonitrile.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69153300 | -0.14155700 | 0.00009300 |
| C | 2.87036700 | 0.70566000 | 0.00046500 |
| C | 3.44688900 | -0.59156800 | 0.00023700 |
| C | 2.59093900 | -1.70104100 | -0.00002400 |
| C | 1.21148100 | -1.50261700 | -0.00006300 |
| C | -0.69156600 | 0.14123500 | -0.00000600 |
| C | -1.21137200 | 1.50233700 | 0.00010000 |
| C | -2.59080500 | 1.70091800 | 0.00013300 |
| C | -3.44687500 | 0.59153700 | -0.00001600 |
| C | -2.87049100 | -0.70575300 | -0.00020800 |
| H | 3.50682700 | 1.58182600 | 0.00068600 |
| H | 2.98532900 | -2.70887800 | -0.00015400 |
| H | -2.98508400 | 2.70879900 | 0.00023100 |
| H | -3.50704500 | -1.58185100 | -0.00033900 |
| O | -0.39424700 | 2.54070400 | 0.00007700 |
| H | 0.55865700 | 2.16515500 | -0.00028300 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.39450800 | -2.54109800 | -0.00016400 |
| H | -0.55845200 | -2.16567300 | 0.00008700 |
| N | 1.57049600 | 0.91876000 | 0.00039500 |
| N | -1.57064100 | -0.91899200 | -0.00019100 |
| C | -4.90378200 | 0.80335400 | 0.00000400 |
| C | 4.90381800 | -0.80323000 | 0.00030000 |
| O | 5.43221100 | -1.90122100 | -0.00018600 |
| O | -5.43205700 | 1.90140200 | 0.00015100 |
| C | -7.04330500 | -0.24956900 | -0.00012700 |
| C | -7.59625800 | -1.65692300 | -0.00026900 |
| H | -7.35354700 | 0.31144800 | -0.88531400 |
| H | -7.35352800 | 0.31126300 | 0.88518400 |
| H | -7.26952800 | -2.20351800 | 0.88802800 |
| H | -8.68897900 | -1.61963300 | -0.00026600 |
| H | -7.26952900 | -2.20333700 | -0.88867900 |
| C | 7.04322900 | 0.24992400 | -0.00015300 |
| C | 7.59602900 | 1.65733800 | -0.00024200 |
| H | 7.35331700 | -0.31094200 | -0.88549000 |
| H | 7.35372700 | -0.31099300 | 0.88500800 |
| H | 7.26945400 | 2.20378000 | 0.88820600 |
| H | 8.68875400 | 1.62016600 | -0.00050500 |
| H | 7.26902800 | 2.20383300 | -0.88850100 |
| O | 5.59473200 | 0.35570900 | 0.00019200 |
| O | -5.59481900 | -0.35551100 | -0.00015300 |

The geometric structure coordinates of T1*/T2* in acetonitrile.

| | | | |
|---|------------|-------------|-------------|
| C | 0.68089800 | 0.11625600 | 0.00003200 |
| C | 2.93607100 | -0.72412400 | -0.00008400 |
| C | 3.46513400 | 0.56561800 | 0.00007100 |
| C | 2.57799700 | 1.66056600 | 0.00020100 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.19912600 | 1.45351000 | 0.00018200 |
| C | -0.71836800 | -0.19581300 | 0.00001200 |
| C | -1.23134900 | -1.58393300 | -0.00011400 |
| C | -2.64665900 | -1.72750000 | -0.00015400 |
| C | -3.48124100 | -0.60684900 | -0.00006400 |
| C | -2.88980900 | 0.66969700 | 0.00008000 |
| H | 3.54835600 | -1.61388500 | -0.00019100 |
| H | 2.95960800 | 2.67297600 | 0.00031700 |
| H | -3.06013700 | -2.72825100 | -0.00025200 |
| H | -3.50144300 | 1.56251300 | 0.00016900 |
| O | -0.44203600 | -2.57273500 | -0.00019200 |
| H | 1.20721600 | -1.85127600 | -0.00018600 |
| O | 0.38768600 | 2.50461500 | 0.00030600 |
| H | -0.55719100 | 2.13723900 | 0.00026100 |
| N | 1.61927300 | -0.90620600 | -0.00010000 |
| N | -1.56722100 | 0.85935500 | 0.00011300 |
| C | -4.94858500 | -0.78920400 | -0.00011400 |
| C | 4.92213400 | 0.80937500 | 0.00008900 |
| O | 5.41869800 | 1.91948700 | 0.00021600 |
| O | -5.49723600 | -1.87491500 | -0.00018700 |
| C | -7.06746000 | 0.30381800 | -0.00002300 |
| C | -7.59202200 | 1.72198900 | 0.00004500 |
| H | -7.38836900 | -0.25062700 | 0.88527100 |
| H | -7.38836400 | -0.25054100 | -0.88537100 |
| H | -7.25453300 | 2.26193600 | -0.88829400 |
| H | -8.68528500 | 1.70657300 | 0.00004400 |
| H | -7.25453400 | 2.26185200 | 0.88843500 |
| C | 7.08362800 | -0.19700800 | -0.00005200 |
| C | 7.66255200 | -1.59350600 | -0.00016200 |
| H | 7.38089300 | 0.36950600 | 0.88574700 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.38087400 | 0.36963700 | -0.88577400 |
| H | 7.34652200 | -2.14585400 | -0.88870400 |
| H | 8.75428000 | -1.53480600 | -0.00017100 |
| H | 7.34654400 | -2.14598200 | 0.88830800 |
| O | 5.63530200 | -0.33133800 | -0.00004900 |
| O | -5.61630000 | 0.38108400 | -0.00001500 |

The geometric structure coordinates of T3* in acetonitrile.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.68219400 | 0.16595800 | 0.00001800 |
| C | 2.93337000 | -0.69457800 | -0.00008400 |
| C | 3.47980500 | 0.59119600 | 0.00004600 |
| C | 2.62046300 | 1.69489400 | 0.00015700 |
| C | 1.20293500 | 1.54648900 | 0.00014100 |
| C | -0.68220000 | -0.16586200 | 0.00000700 |
| C | -1.20289600 | -1.54640600 | -0.00009100 |
| C | -2.62042400 | -1.69485600 | -0.00012200 |
| C | -3.47979900 | -0.59118600 | -0.00005800 |
| C | -2.93339900 | 0.69460600 | 0.00006200 |
| H | 3.53292100 | -1.59262000 | -0.00018400 |
| H | 3.02239300 | 2.70011400 | 0.00025400 |
| H | -3.02232200 | -2.70008900 | -0.00019800 |
| H | -3.53298000 | 1.59262800 | 0.00013300 |
| O | -0.41907500 | -2.53660000 | -0.00012700 |
| H | 1.18703400 | -1.80579900 | -0.00018000 |
| O | 0.41916000 | 2.53672600 | 0.00023800 |
| H | -1.18707500 | 1.80587900 | 0.00016300 |
| N | 1.60912700 | -0.86241500 | -0.00009900 |
| N | -1.60916300 | 0.86248200 | 0.00009500 |
| C | -4.94603000 | -0.80259800 | -0.00011200 |
| C | 4.94604100 | 0.80256400 | 0.00005800 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.46919300 | 1.89897000 | 0.00018100 |
| O | -5.46915100 | -1.89901900 | -0.00015000 |
| C | -7.08428500 | 0.25267800 | 0.00000300 |
| C | -7.63124000 | 1.66203500 | 0.00006900 |
| H | -7.39436400 | -0.30701200 | 0.88566800 |
| H | -7.39437400 | -0.30693400 | -0.88570900 |
| H | -7.30281200 | 2.20720800 | -0.88841600 |
| H | -8.72404400 | 1.62825600 | 0.00008000 |
| H | -7.30279300 | 2.20713200 | 0.88859400 |
| C | 7.08426100 | -0.25278600 | -0.00003700 |
| C | 7.63116500 | -1.66216400 | -0.00012900 |
| H | 7.39436100 | 0.30679500 | 0.88568900 |
| H | 7.39436700 | 0.30691200 | -0.88568800 |
| H | 7.30270800 | -2.20722900 | -0.88867000 |
| H | 8.72397000 | -1.62842300 | -0.00012400 |
| H | 7.30270500 | -2.20734400 | 0.88834100 |
| O | 5.63304100 | -0.35381100 | -0.00005100 |
| O | -5.63306800 | 0.35375200 | -0.00000200 |

The geometric structure coordinates of TS* of N*-T1*/T2* path in acetonitrile.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.67734070 | 0.21349285 | -0.00000156 |
| C | 2.84933170 | -0.69681015 | -0.00005456 |
| C | 3.44007770 | 0.58737185 | 0.00003944 |
| C | 2.60120070 | 1.71681185 | 0.00011044 |
| C | 1.21945770 | 1.55086585 | 0.00009144 |
| C | -0.70441230 | -0.07464015 | -0.00001856 |
| C | -1.17935030 | -1.46202215 | -0.00010956 |
| C | -2.56290630 | -1.68848415 | -0.00012156 |
| C | -3.43693030 | -0.59553415 | -0.00004656 |
| C | -2.89140830 | 0.71435585 | 0.00004044 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.45846670 | -1.59106015 | -0.00011456 |
| H | 3.02055170 | 2.71443685 | 0.00017944 |
| H | -2.93722630 | -2.70406715 | -0.00018856 |
| H | -3.54981830 | 1.57396585 | 0.00010144 |
| O | -0.31635730 | -2.43623315 | -0.00017456 |
| H | 0.72446570 | -1.91720615 | -0.00014356 |
| O | 0.41826270 | 2.60905885 | 0.00015744 |
| H | -0.53069930 | 2.26293485 | 0.00013544 |
| N | 1.54240170 | -0.86423815 | -0.00007256 |
| N | -1.59178230 | 0.96545585 | 0.00005344 |
| C | -4.89227830 | -0.83492315 | -0.00005656 |
| C | 4.90033570 | 0.77445985 | 0.00006244 |
| O | 5.44680870 | 1.86344185 | 0.00013944 |
| O | -5.39852630 | -1.94249215 | -0.00012956 |
| C | -7.05173730 | 0.17663885 | 0.00002844 |
| C | -7.63030530 | 1.57361685 | 0.00011344 |
| H | -7.35109330 | -0.38988415 | 0.88537044 |
| H | -7.35110730 | -0.38978215 | -0.88537256 |
| H | -7.31362930 | 2.12602485 | -0.88821656 |
| H | -8.72214330 | 1.51627385 | 0.00011944 |
| H | -7.31361330 | 2.12592385 | 0.88849944 |
| C | 7.02190470 | -0.31459115 | -0.00000056 |
| C | 7.55078170 | -1.73117915 | -0.00007756 |
| H | 7.34162770 | 0.24083585 | 0.88527544 |
| H | 7.34163170 | 0.24093185 | -0.88521556 |
| H | 7.21486770 | -2.27202515 | -0.88847356 |
| H | 8.64398870 | -1.71251015 | -0.00007556 |
| H | 7.21486570 | -2.27212115 | 0.88826044 |
| O | 5.57166670 | -0.39587615 | -0.00000956 |
| O | -5.60506930 | 0.30962285 | 0.00002544 |

The geometric structure coordinates of TS* of T1*/T2*-T3* path in acetonitrile.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.68832855 | -0.04162409 | -0.00001282 |
| C | 2.95836955 | 0.73548391 | 0.00004118 |
| C | 3.44858555 | -0.57247909 | -0.00002982 |
| C | 2.54204155 | -1.64701009 | -0.00009082 |
| C | 1.15659355 | -1.41389609 | -0.00008282 |
| C | -0.68919845 | 0.27309591 | -0.00000282 |
| C | -1.23300945 | 1.64239791 | 0.00006918 |
| C | -2.65333645 | 1.74748191 | 0.00008618 |
| C | -3.46491545 | 0.60665891 | 0.00003118 |
| C | -2.85790345 | -0.66120809 | -0.00004782 |
| H | 3.59806755 | 1.60557991 | 0.00009318 |
| H | 2.90281355 | -2.66723609 | -0.00014382 |
| H | -3.09440245 | 2.73627391 | 0.00014218 |
| H | -3.44192145 | -1.57112809 | -0.00009982 |
| O | -0.45853245 | 2.64018191 | 0.00011318 |
| H | 1.26359155 | 1.91361891 | 0.00009518 |
| O | 0.29445555 | -2.38762109 | -0.00013582 |
| H | -0.76856045 | -1.83310909 | -0.00010882 |
| N | 1.64547255 | 0.95931291 | 0.00004818 |
| N | -1.53298845 | -0.80322009 | -0.00006282 |
| C | -4.93606845 | 0.75774291 | 0.00005118 |
| C | 4.90258555 | -0.84885909 | -0.00003982 |
| O | 5.37464155 | -1.96883509 | -0.00010082 |
| O | -5.50758545 | 1.83125891 | 0.00011718 |
| C | -7.03040045 | -0.38281109 | -0.00000282 |
| C | -7.52237545 | -1.81258909 | -0.00007482 |
| H | -7.36357845 | 0.16418691 | -0.88536282 |
| H | -7.36357245 | 0.16409591 | 0.88541618 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.17270645 | -2.34468609 | 0.88829518 |
| H | -8.61569445 | -1.82204909 | -0.00007282 |
| H | -7.17270945 | -2.34459509 | -0.88849982 |
| C | 7.08599455 | 0.10959291 | 0.00002018 |
| C | 7.69472555 | 1.49333091 | 0.00008818 |
| H | 7.37066055 | -0.46325409 | -0.88580982 |
| H | 7.37065455 | -0.46333809 | 0.88579818 |
| H | 7.39065055 | 2.05234991 | 0.88862718 |
| H | 8.78492655 | 1.41118491 | 0.00008918 |
| H | 7.39065755 | 2.05243391 | -0.88840082 |
| O | 5.64069755 | 0.27523491 | 0.00002418 |
| O | -5.57766645 | -0.42703009 | -0.00001082 |

The geometric structure coordinates of N under $E_x = 0$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.71970200 | 0.15199500 | -0.00006300 |
| C | 2.88062100 | -0.71668000 | 0.00023100 |
| C | 3.44486500 | 0.56410800 | 0.00009200 |
| C | 2.60014600 | 1.66674000 | -0.00015200 |
| C | 1.21578500 | 1.48649300 | -0.00024800 |
| C | -0.71971000 | -0.15189400 | -0.00007700 |
| C | -1.21575100 | -1.48640800 | 0.00009600 |
| C | -2.60010600 | -1.66670000 | 0.00000700 |
| C | -3.44486200 | -0.56409700 | -0.00022100 |
| C | -2.88065900 | 0.71670900 | -0.00035100 |
| H | 3.50495000 | -1.60019000 | 0.00041700 |
| H | 3.00799100 | 2.66955800 | -0.00029400 |
| H | -3.00791800 | -2.66953100 | 0.00013200 |
| H | -3.50501700 | 1.60019800 | -0.00052300 |
| O | -0.42792200 | -2.56420300 | 0.00034100 |
| H | 0.51145900 | -2.22947200 | 0.00054900 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.42799700 | 2.56431700 | -0.00054900 |
| H | -0.51139100 | 2.22960900 | -0.00071900 |
| N | 1.56661100 | -0.90076800 | 0.00014600 |
| N | -1.56665400 | 0.90084100 | -0.00028300 |
| C | -4.91872800 | -0.79486800 | -0.00027100 |
| C | 4.91873700 | 0.79483200 | 0.00018600 |
| O | 5.43292800 | 1.88760900 | 0.00008200 |
| O | -5.43288200 | -1.88766200 | -0.00001600 |
| C | -7.05623800 | 0.23839900 | -0.00063300 |
| C | -7.62233900 | 1.64255600 | 0.00169200 |
| H | -7.35763300 | -0.33280000 | 0.88077800 |
| H | -7.35796300 | -0.32992100 | -0.88382700 |
| H | -7.29604500 | 2.19268400 | -0.88349700 |
| H | -8.71452300 | 1.60298000 | 0.00114500 |
| H | -7.29679100 | 2.18952000 | 0.88911700 |
| C | 7.05621500 | -0.23850900 | 0.00043100 |
| C | 7.62227600 | -1.64268500 | -0.00045500 |
| H | 7.35776400 | 0.33064700 | 0.88313100 |
| H | 7.35781900 | 0.33183700 | -0.88147600 |
| H | 7.29586400 | -2.19077000 | -0.88686600 |
| H | 8.71446000 | -1.60314200 | -0.00102300 |
| H | 7.29680800 | -2.19167100 | 0.88575200 |
| O | 5.61092500 | -0.36020500 | 0.00044100 |
| O | -5.61095400 | 0.36014500 | -0.00072700 |

The geometric structure coordinates of N* under $E_x = 0$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.69836100 | 0.14243300 | 0.00005700 |
| C | 2.87503200 | -0.70515600 | -0.00027500 |
| C | 3.45299100 | 0.58692300 | 0.00004100 |
| C | 2.59844400 | 1.69638600 | 0.00031100 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.21784300 | 1.49821200 | 0.00028300 |
| C | -0.69835000 | -0.14253200 | 0.00010400 |
| C | -1.21787700 | -1.49830000 | -0.00008600 |
| C | -2.59848600 | -1.69642400 | -0.00017000 |
| C | -3.45299500 | -0.58693200 | 0.00001800 |
| C | -2.87499200 | 0.70512600 | 0.00030200 |
| H | 3.51334900 | -1.57983200 | -0.00049600 |
| H | 2.99909600 | 2.70133000 | 0.00050200 |
| H | -2.99917400 | -2.70135400 | -0.00033100 |
| H | -3.51327900 | 1.57982400 | 0.00045800 |
| O | -0.40514600 | -2.54262200 | -0.00007900 |
| H | 0.54568600 | -2.17467600 | 0.00032800 |
| O | 0.40506100 | 2.54249600 | 0.00037500 |
| H | -0.54574700 | 2.17450400 | 0.00004400 |
| N | 1.57070200 | -0.91698000 | -0.00026200 |
| N | -1.57065400 | 0.91690800 | 0.00033600 |
| C | -4.91079300 | -0.80191300 | -0.00005100 |
| C | 4.91078200 | 0.80195300 | 0.00006200 |
| O | 5.44014200 | 1.89373700 | 0.00035200 |
| O | -5.44019100 | -1.89367900 | -0.00041900 |
| C | -7.04337800 | 0.24666900 | -0.00024100 |
| C | -7.60918800 | 1.65157300 | 0.00047400 |
| H | -7.34953000 | -0.32307000 | 0.88112800 |
| H | -7.34936200 | -0.32207600 | -0.88231900 |
| H | -7.28233900 | 2.20052900 | -0.88543700 |
| H | -8.70154500 | 1.61395100 | 0.00030700 |
| H | -7.28257200 | 2.19952600 | 0.88709100 |
| C | 7.04340200 | -0.24655700 | -0.00012400 |
| C | 7.60925900 | -1.65144300 | -0.00066200 |
| H | 7.34945200 | 0.32235400 | 0.88182100 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.34944900 | 0.32303500 | -0.88162700 |
| H | 7.28254500 | -2.19956500 | -0.88713900 |
| H | 8.70161400 | -1.61378400 | -0.00064600 |
| H | 7.28254400 | -2.20025100 | 0.88538900 |
| O | 5.60194900 | -0.36574600 | -0.00016200 |
| O | -5.60192200 | 0.36580900 | -0.00004700 |

The geometric structure coordinates of T1*/T2* under $E_x = 0$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.68479900 | 0.16701400 | 0.14076100 |
| C | -2.93168500 | -0.70643600 | 0.16394500 |
| C | -3.46116000 | 0.55600200 | -0.01428000 |
| C | -2.58908900 | 1.66640600 | -0.09711800 |
| C | -1.21217700 | 1.48013500 | -0.01245400 |
| C | 0.73162800 | -0.13574500 | 0.04469700 |
| C | 1.22200500 | -1.51503800 | -0.10409100 |
| C | 2.61186100 | -1.68321200 | -0.07863200 |
| C | 3.47302800 | -0.57364400 | -0.00626200 |
| C | 2.91986500 | 0.69867700 | 0.07250200 |
| H | -3.54307300 | -1.59117300 | 0.25554200 |
| H | -2.99020100 | 2.66436800 | -0.20310300 |
| H | 3.01913600 | -2.67712700 | -0.20506800 |
| H | 3.53726600 | 1.58636600 | 0.06388400 |
| O | 0.38142000 | -2.47928400 | -0.20029700 |
| H | -1.19086300 | -1.80496400 | 0.29375100 |
| O | -0.41269100 | 2.54587500 | -0.07550300 |
| H | 0.52105100 | 2.22442700 | 0.04173400 |
| N | -1.60198400 | -0.86555000 | 0.27649600 |
| N | 1.59483000 | 0.87826400 | 0.14637100 |
| C | 4.93644700 | -0.80173200 | -0.05346800 |
| C | -4.92409100 | 0.78107300 | -0.08153900 |

| | | | |
|---|-------------|-------------|-------------|
| O | -5.43358100 | 1.86772600 | -0.23026600 |
| O | 5.45252400 | -1.89112400 | -0.16090900 |
| C | 7.07875000 | 0.22167500 | -0.00240400 |
| C | 7.65586600 | 1.61738600 | 0.10925000 |
| H | 7.36174200 | -0.26986400 | -0.93672600 |
| H | 7.39618900 | -0.42430400 | 0.82011800 |
| H | 7.34971700 | 2.08839300 | 1.04588900 |
| H | 8.74767600 | 1.57250500 | 0.08525200 |
| H | 7.31752100 | 2.24322100 | -0.71947200 |
| C | -7.06836500 | -0.24169900 | -0.03287800 |
| C | -7.64774700 | -1.63230000 | 0.12016200 |
| H | -7.33492100 | 0.21521200 | -0.98917000 |
| H | -7.39753500 | 0.43402400 | 0.76042400 |
| H | -7.35953300 | -2.06838800 | 1.07917500 |
| H | -8.73880500 | -1.58789500 | 0.07521100 |
| H | -7.29600300 | -2.28839000 | -0.67905200 |
| O | -5.62661200 | -0.36895900 | 0.03464100 |
| O | 5.63752600 | 0.35116600 | 0.03763500 |

The geometric structure coordinates of T3* in under $E_x = 0$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.68651200 | -0.16804900 | -0.00003400 |
| C | -2.92805500 | 0.69444200 | -0.00004500 |
| C | -3.46994800 | -0.59228600 | -0.00003700 |
| C | -2.61148600 | -1.69788700 | -0.00002800 |
| C | -1.19711300 | -1.54426200 | -0.00003100 |
| C | 0.68660400 | 0.16797500 | -0.00003200 |
| C | 1.19705900 | 1.54436300 | -0.00004500 |
| C | 2.61150300 | 1.69791900 | -0.00004700 |
| C | 3.46989000 | 0.59229500 | -0.00003700 |
| C | 2.92805700 | -0.69449000 | -0.00002300 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.53867900 | 1.58478300 | -0.00005400 |
| H | -3.01822700 | -2.70041800 | -0.00001700 |
| H | 3.01834100 | 2.70041300 | -0.00005900 |
| H | 3.53882100 | -1.58473800 | -0.00001000 |
| O | 0.39977100 | 2.52810800 | -0.00005800 |
| H | -1.14388200 | 1.80254200 | -0.00004900 |
| O | -0.39975200 | -2.52809000 | -0.00002400 |
| H | 1.14382700 | -1.80275600 | -0.00001400 |
| N | -1.60136100 | 0.86491700 | -0.00004200 |
| N | 1.60143800 | -0.86505700 | -0.00002100 |
| C | 4.93644800 | 0.80641500 | -0.00004100 |
| C | -4.93650700 | -0.80641800 | -0.00003300 |
| O | -5.46393100 | -1.89469300 | -0.00001400 |
| O | 5.46389200 | 1.89468300 | -0.00003700 |
| C | 7.06696800 | -0.24810600 | -0.00000600 |
| C | 7.62649100 | -1.65525800 | 0.00039000 |
| H | 7.37359300 | 0.31995700 | 0.88191100 |
| H | 7.37366300 | 0.31947500 | -0.88221300 |
| H | 7.29831800 | -2.20266100 | -0.88597400 |
| H | 8.71890000 | -1.62159600 | 0.00040500 |
| H | 7.29827600 | -2.20217300 | 0.88704000 |
| C | -7.06700400 | 0.24815100 | -0.00002700 |
| C | -7.62647100 | 1.65532100 | 0.00020300 |
| H | -7.37363900 | -0.31979500 | 0.88196000 |
| H | -7.37369300 | -0.31952600 | -0.88217000 |
| H | -7.29825900 | 2.20261500 | -0.88621300 |
| H | -8.71888300 | 1.62169600 | 0.00019300 |
| H | -7.29826600 | 2.20232100 | 0.88680300 |
| O | -5.62296500 | 0.36135500 | -0.00005700 |
| O | 5.62295100 | -0.36135300 | -0.00004200 |

The geometric structure coordinates of TS* of N*-T1*/T2* path under $E_x = 0$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.68853283 | 0.22821299 | 0.00001491 |
| C | -2.85355483 | -0.69615501 | -0.00008309 |
| C | -3.44892083 | 0.58278099 | 0.00002591 |
| C | -2.61424283 | 1.71455799 | 0.00013291 |
| C | -1.22955083 | 1.55411299 | 0.00012891 |
| C | 0.71394617 | -0.06435401 | 0.00000091 |
| C | 1.18741417 | -1.44953801 | -0.00012009 |
| C | 2.56859417 | -1.67989901 | -0.00013009 |
| C | 3.44671017 | -0.58788001 | -0.00002609 |
| C | 2.90344117 | 0.71184099 | 0.00008691 |
| H | -3.46218183 | -1.59052501 | -0.00016709 |
| H | -3.04294583 | 2.70768799 | 0.00021791 |
| H | 2.94625417 | -2.69380301 | -0.00021809 |
| H | 3.56110717 | 1.57159199 | 0.00016891 |
| O | 0.32133517 | -2.42440901 | -0.00021409 |
| H | -0.72236783 | -1.90112601 | -0.00017509 |
| O | -0.44110083 | 2.62636099 | 0.00022991 |
| H | 0.50407917 | 2.30029799 | 0.00020891 |
| N | -1.54410283 | -0.85425301 | -0.00008709 |
| N | 1.59126917 | 0.96520299 | 0.00009991 |
| C | 4.90295917 | -0.83599701 | -0.00003809 |
| C | -4.90965483 | 0.76848799 | 0.00003191 |
| O | -5.46211383 | 1.84910199 | 0.00012391 |
| O | 5.40401517 | -1.93951901 | -0.00013309 |
| C | 7.05933917 | 0.16225499 | 0.00006591 |
| C | 7.65575617 | 1.55426399 | 0.00019191 |
| H | 7.35171717 | -0.41348401 | -0.88188909 |
| H | 7.35170517 | -0.41363801 | 0.88192391 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.34147117 | 2.10970999 | 0.88655791 |
| H | 8.74695517 | 1.49217799 | 0.00019391 |
| H | 7.34148317 | 2.10986499 | -0.88608009 |
| C | -7.02084783 | -0.32332901 | -0.00008109 |
| C | -7.55891483 | -1.73921001 | -0.00020909 |
| H | -7.33866983 | 0.23958499 | -0.88171909 |
| H | -7.33868283 | 0.23943099 | 0.88164991 |
| H | -7.22136783 | -2.28121001 | 0.88601391 |
| H | -8.65181583 | -1.72341001 | -0.00021609 |
| H | -7.22135483 | -2.28105501 | -0.88652009 |
| O | -5.57779283 | -0.41403601 | -0.00007909 |
| O | 5.61972117 | 0.31354099 | 0.00006991 |

The geometric structure coordinates of TS* of T1*/T2*-T3* path under $E_x = 0$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | -0.69420860 | -0.06879035 | -0.00000879 |
| C | -2.94834560 | 0.72987265 | -0.00001379 |
| C | -3.44501160 | -0.57617035 | 0.00001121 |
| C | -2.54975060 | -1.65758235 | 0.00002621 |
| C | -1.15759160 | -1.43804335 | 0.00001621 |
| C | 0.69543940 | 0.25141565 | -0.00001079 |
| C | 1.22395340 | 1.61583265 | -0.00003079 |
| C | 2.63622140 | 1.73698165 | -0.00003179 |
| C | 3.45792540 | 0.59798865 | -0.00001279 |
| C | 2.86831540 | -0.66992735 | 0.00000621 |
| H | -3.59171160 | 1.59676465 | -0.00002779 |
| H | -2.92582860 | -2.67180435 | 0.00004521 |
| H | 3.07621740 | 2.72541265 | -0.00004479 |
| H | 3.46137240 | -1.57336835 | 0.00002321 |
| O | 0.42588140 | 2.60580365 | -0.00004879 |
| H | -1.19990360 | 1.88625665 | -0.00003979 |

| | | | |
|---|-------------|-------------|-------------|
| O | -0.29862760 | -2.40652635 | 0.00002821 |
| H | 0.79980840 | -1.82869835 | 0.00001721 |
| N | -1.63237660 | 0.94205665 | -0.00002379 |
| N | 1.53511640 | -0.81970735 | 0.00000521 |
| C | 4.92879540 | 0.76787265 | -0.00001179 |
| C | -4.90220560 | -0.84269235 | 0.00002121 |
| O | -5.38875660 | -1.95048235 | 0.00004221 |
| O | 5.48936840 | 1.84063565 | -0.00002579 |
| C | 7.02860840 | -0.34502635 | 0.00001021 |
| C | 7.54938840 | -1.76715735 | 0.00003321 |
| H | 7.35174240 | 0.21402665 | 0.88192021 |
| H | 7.35174740 | 0.21400065 | -0.88191379 |
| H | 7.20567940 | -2.30501735 | -0.88628679 |
| H | 8.64236640 | -1.76401635 | 0.00003521 |
| H | 7.20567440 | -2.30499135 | 0.88636721 |
| C | -7.06937160 | 0.13431965 | 0.00001121 |
| C | -7.67902260 | 1.52039265 | -0.00001079 |
| H | -7.35504160 | -0.44419335 | 0.88214521 |
| H | -7.35504760 | -0.44422435 | -0.88209979 |
| H | -7.37093460 | 2.07897865 | -0.88659479 |
| H | -8.76947160 | 1.44725465 | -0.00000579 |
| H | -7.37092760 | 2.07900965 | 0.88655121 |
| O | -5.62995360 | 0.29932865 | 0.00000321 |
| O | 5.58309140 | -0.41886435 | 0.00000821 |

The geometric structure coordinates of N under $E_x = +1 \times 10^{-4}$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.71986300 | 0.15193500 | -0.00002700 |
| C | 2.88090500 | -0.71636900 | 0.00000700 |
| C | 3.44503300 | 0.56440400 | 0.00015100 |
| C | 2.60011000 | 1.66701100 | 0.00015700 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.21582100 | 1.48661100 | 0.00003500 |
| C | -0.71953700 | -0.15196000 | -0.00001700 |
| C | -1.21568500 | -1.48634200 | -0.00008400 |
| C | -2.60008300 | -1.66646200 | -0.00020300 |
| C | -3.44464000 | -0.56384200 | -0.00019900 |
| C | -2.88030300 | 0.71696800 | -0.00005200 |
| H | 3.50521500 | -1.59989200 | -0.00002400 |
| H | 3.00771900 | 2.66991700 | 0.00021100 |
| H | -3.00816000 | -2.66919100 | -0.00025200 |
| H | -3.50464000 | 1.60046000 | -0.00002100 |
| O | -0.42806200 | -2.56439700 | 0.00003200 |
| H | 0.51122400 | -2.22998600 | 0.00030900 |
| O | 0.42787100 | 2.56422200 | -0.00008800 |
| H | -0.51156500 | 2.22923200 | -0.00037300 |
| N | 1.56691500 | -0.90062200 | -0.00007700 |
| N | -1.56630100 | 0.90094900 | 0.00003700 |
| C | -4.91873500 | -0.79474800 | -0.00029500 |
| C | 4.91870200 | 0.79496600 | 0.00024900 |
| O | 5.43356800 | 1.88745600 | 0.00032300 |
| O | -5.43218000 | -1.88778200 | -0.00029800 |
| C | -7.05633000 | 0.23836900 | -0.00012900 |
| C | -7.62257200 | 1.64243700 | 0.00112000 |
| H | -7.35762800 | -0.33219900 | 0.88171100 |
| H | -7.35786800 | -0.33067800 | -0.88287900 |
| H | -7.29690100 | 2.19179700 | -0.88476800 |
| H | -8.71470800 | 1.60258700 | 0.00114800 |
| H | -7.29679100 | 2.19025300 | 0.88792100 |
| C | 7.05592300 | -0.23859600 | 0.00019400 |
| C | 7.62200800 | -1.64282500 | -0.00041100 |
| H | 7.35775600 | 0.33075800 | 0.88269800 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.35770100 | 0.33150200 | -0.88184200 |
| H | 7.29587100 | -2.19095800 | -0.88688900 |
| H | 8.71422000 | -1.60341200 | -0.00044900 |
| H | 7.29595800 | -2.19169900 | 0.88563800 |
| O | 5.61096100 | -0.36030400 | 0.00018700 |
| O | -5.61081700 | 0.36003300 | -0.00025700 |

The geometric structure coordinates of N* under $E_x = +1 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69855000 | 0.14412400 | 0.00001900 |
| C | 2.87499600 | -0.70435000 | -0.00004800 |
| C | 3.45331200 | 0.58780300 | 0.00012000 |
| C | 2.59880500 | 1.69753300 | 0.00027600 |
| C | 1.21811700 | 1.49947300 | 0.00024500 |
| C | -0.69819100 | -0.14087700 | -0.00005500 |
| C | -1.21732300 | -1.49713500 | -0.00028600 |
| C | -2.59783800 | -1.69582700 | -0.00026200 |
| C | -3.45259300 | -0.58670000 | -0.00007600 |
| C | -2.87528100 | 0.70536500 | 0.00007600 |
| H | 3.51310800 | -1.57917600 | -0.00017700 |
| H | 2.99947300 | 2.70244200 | 0.00043600 |
| H | -2.99821400 | -2.70088700 | -0.00041300 |
| H | -3.51385000 | 1.57984500 | 0.00022000 |
| O | -0.40396800 | -2.54079100 | -0.00057400 |
| H | 0.54691600 | -2.17175200 | -0.00074100 |
| O | 0.40573100 | 2.54424800 | 0.00048100 |
| H | -0.54500800 | 2.17701000 | 0.00061900 |
| N | 1.57094700 | -0.91578300 | -0.00010100 |
| N | -1.57061300 | 0.91785800 | 0.00009100 |
| C | -4.91068300 | -0.80250800 | -0.00006000 |
| C | 4.91073100 | 0.80217000 | 0.00015100 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.44127600 | 1.89356400 | 0.00029700 |
| O | -5.43866100 | -1.89476500 | -0.00014700 |
| C | -7.04382000 | 0.24514100 | 0.00028600 |
| C | -7.60986300 | 1.64987600 | 0.00060000 |
| H | -7.34939600 | -0.32437000 | 0.88195800 |
| H | -7.34954400 | -0.32403400 | -0.88155300 |
| H | -7.28348000 | 2.19858500 | -0.88562800 |
| H | -8.70217800 | 1.61186100 | 0.00068600 |
| H | -7.28333000 | 2.19824900 | 0.88698100 |
| C | 7.04273900 | -0.24754800 | -0.00002600 |
| C | 7.60810800 | -1.65270600 | -0.00025300 |
| H | 7.34932600 | 0.32139600 | 0.88175500 |
| H | 7.34930500 | 0.32167400 | -0.88163500 |
| H | 7.28102800 | -2.20089400 | -0.88656200 |
| H | 8.70050900 | -1.61561600 | -0.00025400 |
| H | 7.28103900 | -2.20117500 | 0.88588600 |
| O | 5.60163800 | -0.36625900 | -0.00002700 |
| O | -5.60198700 | 0.36453900 | 0.00018600 |

The geometric structure coordinates of T1* under $E_x = +1 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.67230400 | 0.16026800 | -0.12103800 |
| C | 2.91475400 | -0.72317100 | -0.13891800 |
| C | 3.44973100 | 0.53875300 | 0.02810100 |
| C | 2.58273700 | 1.65354000 | 0.10282400 |
| C | 1.20447800 | 1.47180000 | 0.02121200 |
| C | -0.74596200 | -0.13707200 | -0.02087300 |
| C | -1.23884600 | -1.51315000 | 0.14445600 |
| C | -2.62981700 | -1.67763700 | 0.12065100 |
| C | -3.48762900 | -0.56674300 | 0.03581100 |
| C | -2.93123200 | 0.70311500 | -0.05709800 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.52254400 | -1.61109000 | -0.22336700 |
| H | 2.98793800 | 2.65075700 | 0.19961900 |
| H | -3.03985000 | -2.66888600 | 0.25886900 |
| H | -3.54615700 | 1.59252800 | -0.05794200 |
| O | -0.40178900 | -2.47868900 | 0.25343100 |
| H | 1.16843000 | -1.81549300 | -0.25375100 |
| O | 0.40926800 | 2.54113800 | 0.07606700 |
| H | -0.52568200 | 2.22273100 | -0.03997900 |
| N | 1.58448100 | -0.87774600 | -0.24919600 |
| N | -1.60513500 | 0.87845000 | -0.13383400 |
| C | -4.95218600 | -0.79058500 | 0.08527200 |
| C | 4.91363100 | 0.75767900 | 0.09172800 |
| O | 5.42872900 | 1.84296200 | 0.23126300 |
| O | -5.47036700 | -1.87752800 | 0.20512800 |
| C | -7.09190100 | 0.23757700 | 0.02066100 |
| C | -7.66510600 | 1.63328200 | -0.10891600 |
| H | -7.37655600 | -0.24144400 | 0.96092400 |
| H | -7.41027400 | -0.41787300 | -0.79391700 |
| H | -7.35719200 | 2.09164700 | -1.05122400 |
| H | -8.75701900 | 1.59152400 | -0.08510200 |
| H | -7.32575200 | 2.26858600 | 0.71214700 |
| C | 7.05309400 | -0.27520000 | 0.04945700 |
| C | 7.62620500 | -1.66963700 | -0.09239900 |
| H | 7.32267300 | 0.18848300 | 1.00166600 |
| H | 7.38482700 | 0.39236600 | -0.74970500 |
| H | 7.33510700 | -2.11245100 | -1.04745500 |
| H | 8.71751400 | -1.62981400 | -0.04873100 |
| H | 7.27211900 | -2.31742100 | 0.71253700 |
| O | 5.61104600 | -0.39664000 | -0.01587300 |
| O | -5.64992600 | 0.36260400 | -0.02000900 |

The geometric structure coordinates of T2* under $E_x = +1 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.74596600 | 0.14083500 | 0.02393300 |
| C | 2.93111900 | -0.70087700 | 0.05970500 |
| C | 3.48899400 | 0.56853700 | -0.03284400 |
| C | 2.63166600 | 1.68040800 | -0.11631200 |
| C | 1.24110900 | 1.51674300 | -0.13951300 |
| C | -0.67151800 | -0.15595300 | 0.12359300 |
| C | -1.20339100 | -1.46860500 | -0.01637700 |
| C | -2.58106900 | -1.65101900 | -0.09884300 |
| C | -3.44912600 | -0.53700200 | -0.02681800 |
| C | -2.91543900 | 0.72535100 | 0.13893500 |
| H | 3.54534400 | -1.59081600 | 0.06012000 |
| H | 3.04221600 | 2.67153100 | -0.25360400 |
| H | -2.98562900 | -2.64860100 | -0.19488800 |
| H | -3.52393000 | 1.61292200 | 0.22205100 |
| O | -0.40775400 | -2.53782000 | -0.06929000 |
| H | 0.52710600 | -2.21866700 | 0.04498800 |
| O | 0.40413800 | 2.48288500 | -0.24614100 |
| H | -1.17098700 | 1.81924700 | 0.25700500 |
| N | 1.60551300 | -0.87530800 | 0.13602900 |
| N | -1.58506400 | 0.88113300 | 0.24965300 |
| C | -4.91313100 | -0.75805200 | -0.09159300 |
| C | 4.95293900 | 0.79042800 | -0.08333700 |
| O | 5.47373500 | 1.87648800 | -0.20204000 |
| O | -5.42552800 | -1.84467600 | -0.22948800 |
| C | -7.05418600 | 0.27200800 | -0.05263700 |
| C | -7.62885500 | 1.66594100 | 0.08665200 |
| H | -7.38509800 | -0.39468600 | 0.74750800 |
| H | -7.32232800 | -0.19359100 | -1.00424800 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.27533600 | 2.31285200 | -0.71922800 |
| H | -8.72004300 | 1.62459100 | 0.04247100 |
| H | -7.33900900 | 2.11065200 | 1.04120100 |
| C | 7.09126000 | -0.24066800 | -0.02289500 |
| C | 7.66325700 | -1.63735100 | 0.10285300 |
| H | 7.41183700 | 0.41255900 | 0.79269600 |
| H | 7.37574900 | 0.24008700 | -0.96239300 |
| H | 7.32195700 | -2.27041000 | -0.71914700 |
| H | 8.75524100 | -1.59693900 | 0.07780800 |
| H | 7.35575500 | -2.09750400 | 1.04443400 |
| O | 5.64990400 | -0.36440500 | 0.01929100 |
| O | -5.61165700 | 0.39508100 | 0.01319400 |

The geometric structure coordinates of T3* in under $E_x = +1 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.68757400 | 0.16747100 | -0.00023000 |
| C | 2.93019900 | -0.70068100 | -0.00020900 |
| C | 3.47682600 | 0.58355400 | -0.00004200 |
| C | 2.62120500 | 1.69068200 | -0.00001400 |
| C | 1.20552800 | 1.54260400 | -0.00022500 |
| C | -0.68736200 | -0.16624000 | -0.00006700 |
| C | -1.20509900 | -1.54149400 | -0.00009900 |
| C | -2.62074900 | -1.68945400 | -0.00018900 |
| C | -3.47624800 | -0.58250100 | -0.00011700 |
| C | -2.93007000 | 0.70168700 | 0.00001700 |
| H | 3.53693200 | -1.59365200 | -0.00026800 |
| H | 3.02983500 | 2.69244400 | 0.00006100 |
| H | -3.02961400 | -2.69113900 | -0.00022400 |
| H | -3.53698200 | 1.59454800 | 0.00007300 |
| O | -0.41660500 | -2.53113700 | -0.00005300 |
| H | 1.15315600 | -1.80398700 | -0.00033100 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.41705300 | 2.53222800 | -0.00033700 |
| H | -1.15269500 | 1.80510400 | 0.00003300 |
| N | 1.60273600 | -0.86646000 | -0.00031200 |
| N | -1.60230100 | 0.86758100 | 0.00004800 |
| C | -4.94382100 | -0.79245900 | -0.00014400 |
| C | 4.94387100 | 0.79252300 | 0.00009100 |
| O | 5.47569700 | 1.87868700 | 0.00021300 |
| O | -5.47374500 | -1.87932500 | -0.00013700 |
| C | -7.07121500 | 0.26849600 | -0.00006200 |
| C | -7.62618100 | 1.67737800 | 0.00121400 |
| H | -7.37929800 | -0.29918800 | 0.88154200 |
| H | -7.37951300 | -0.29756900 | -0.88264200 |
| H | -7.29631600 | 2.22432100 | -0.88480600 |
| H | -8.71866500 | 1.64707400 | 0.00108700 |
| H | -7.29645200 | 2.22267500 | 0.88828800 |
| C | 7.07047700 | -0.26973700 | 0.00019700 |
| C | 7.62508300 | -1.67888800 | -0.00005600 |
| H | 7.37926000 | 0.29678500 | 0.88238900 |
| H | 7.37940200 | 0.29715300 | -0.88170400 |
| H | 7.29488000 | -2.22469200 | -0.88665600 |
| H | 8.71763000 | -1.64919000 | -0.00000700 |
| H | 7.29480900 | -2.22505300 | 0.88629400 |
| O | 5.62635600 | -0.37796400 | 0.00006600 |
| O | -5.62644900 | 0.37706200 | -0.00018700 |

The geometric structure coordinates of TS* of N*-T1* path under $E_x = +1 \times 10^{-4}$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.69844800 | 0.24796200 | 0.00002200 |
| C | 2.86278400 | -0.67792300 | -0.00016700 |
| C | 3.45908600 | 0.60074400 | 0.00013000 |
| C | 2.62485400 | 1.73306100 | 0.00036000 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.24000000 | 1.57330700 | 0.00031000 |
| C | -0.70471400 | -0.04425600 | 0.00002700 |
| C | -1.17854700 | -1.42939600 | -0.00014800 |
| C | -2.55979200 | -1.65924200 | -0.00016300 |
| C | -3.43753900 | -0.56702300 | 0.00001400 |
| C | -2.89416200 | 0.73220100 | 0.00020900 |
| H | 3.47076800 | -1.57272500 | -0.00037400 |
| H | 3.05395400 | 2.72600300 | 0.00057300 |
| H | -2.93787400 | -2.67300500 | -0.00029100 |
| H | -3.55137300 | 1.59227400 | 0.00037200 |
| O | -0.31280800 | -2.40452000 | -0.00026700 |
| H | 0.73129400 | -1.88144300 | -0.00037000 |
| O | 0.45229600 | 2.64620000 | 0.00053700 |
| H | -0.49317800 | 2.32089500 | 0.00045200 |
| N | 1.55340200 | -0.83503900 | -0.00022900 |
| N | -1.58130100 | 0.98510000 | 0.00021100 |
| C | -4.89424500 | -0.81518000 | 0.00001000 |
| C | 4.91954500 | 0.78529600 | 0.00017900 |
| O | 5.47357000 | 1.86529700 | 0.00042700 |
| O | -5.39456500 | -1.91885800 | -0.00014100 |
| C | -7.05064800 | 0.18317700 | 0.00021300 |
| C | -7.64662200 | 1.57530200 | 0.00045800 |
| H | -7.34286300 | -0.39273600 | 0.88206100 |
| H | -7.34291400 | -0.39244600 | -0.88180800 |
| H | -7.33236800 | 2.13089200 | -0.88582100 |
| H | -8.73780200 | 1.51338000 | 0.00048200 |
| H | -7.33231200 | 2.13060200 | 0.88689800 |
| C | 7.02982000 | -0.30821000 | -0.00005600 |
| C | 7.56707800 | -1.72447400 | -0.00037700 |
| H | 7.34827300 | 0.25417600 | 0.88173800 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.34828200 | 0.25457900 | -0.88159000 |
| H | 7.22901900 | -2.26597000 | -0.88672100 |
| H | 8.66001700 | -1.70952300 | -0.00037200 |
| H | 7.22901700 | -2.26637300 | 0.88571900 |
| O | 5.58709500 | -0.39811800 | -0.00008400 |
| O | -5.61060000 | 0.33403500 | 0.00019500 |

The geometric structure coordinates of TS* of T1*-T3* path under $E_x = +1 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69449980 | 0.06814377 | -0.00062381 |
| C | 2.94627880 | -0.73661023 | -0.00180581 |
| C | 3.44656180 | 0.56820977 | -0.00144481 |
| C | 2.55405580 | 1.65206877 | -0.00066381 |
| C | 1.16129880 | 1.43607777 | -0.00027781 |
| C | -0.69621320 | -0.24870923 | 0.00002819 |
| C | -1.22756820 | -1.61198123 | -0.00008681 |
| C | -2.64005520 | -1.72986823 | 0.00067119 |
| C | -3.45909620 | -0.58903023 | 0.00149619 |
| C | -2.86693520 | 0.67745277 | 0.00151419 |
| H | 3.58726680 | -1.60525223 | -0.00243481 |
| H | 2.93270580 | 2.66532277 | -0.00041081 |
| H | -3.08247020 | -2.71723023 | 0.00067519 |
| H | -3.45794920 | 1.58221877 | 0.00213319 |
| O | -0.43154920 | -2.60369423 | -0.00087481 |
| H | 1.19441780 | -1.88822223 | -0.00156781 |
| O | 0.30472280 | 2.40670177 | 0.00037719 |
| H | -0.79516920 | 1.83166877 | 0.00068619 |
| N | 1.62991580 | -0.94519823 | -0.00139681 |
| N | -1.53306920 | 0.82417577 | 0.00076719 |
| C | -4.93067720 | -0.75612923 | 0.00234519 |
| C | 4.90417380 | 0.83048177 | -0.00190281 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.39456680 | 1.93670377 | -0.00162081 |
| O | -5.49266020 | -1.82801923 | 0.00239619 |
| C | -7.02842120 | 0.36075877 | 0.00389219 |
| C | -7.54621720 | 1.78391377 | 0.00375319 |
| H | -7.35196120 | -0.19737723 | 0.88619619 |
| H | -7.35295520 | -0.19793523 | -0.87768581 |
| H | -7.20215820 | 2.32075077 | -0.88304681 |
| H | -8.63917320 | 1.78289577 | 0.00453319 |
| H | -7.20089920 | 2.32138277 | 0.88968019 |
| C | 7.06842480 | -0.15280723 | -0.00316381 |
| C | 7.67432780 | -1.54058923 | -0.00392581 |
| H | 7.35627380 | 0.42457477 | 0.87904219 |
| H | 7.35559280 | 0.42524377 | -0.88515281 |
| H | 7.36421780 | -2.09800223 | -0.89054881 |
| H | 8.76500480 | -1.47056723 | -0.00433281 |
| H | 7.36492180 | -2.09866823 | 0.88252519 |
| O | 5.62891480 | -0.31392423 | -0.00266981 |
| O | -5.58240320 | 0.43154377 | 0.00307119 |

The geometric structure coordinates of TS* of N*-T2* path under $E_x = +1 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.71374374 | 0.06479637 | 0.00002333 |
| C | 2.90282774 | -0.71264763 | -0.00017267 |
| C | 3.44693774 | 0.58714137 | 0.00006133 |
| C | 2.56922774 | 1.67956437 | 0.00027433 |
| C | 1.18788974 | 1.44976437 | 0.00025133 |
| C | -0.68830126 | -0.22718863 | 0.00001333 |
| C | -1.22987226 | -1.55315663 | -0.00026667 |
| C | -2.61455226 | -1.71312863 | -0.00030267 |
| C | -3.44878826 | -0.58123163 | -0.00006367 |
| C | -2.85334126 | 0.69746937 | 0.00021733 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.56027474 | -1.57258763 | -0.00035667 |
| H | 2.94717974 | 2.69334637 | 0.00044133 |
| H | -3.04364626 | -2.70610563 | -0.00051067 |
| H | -3.46184526 | 1.59192537 | 0.00042033 |
| O | -0.44168326 | -2.62549063 | -0.00049867 |
| H | 0.50365774 | -2.29950963 | -0.00043067 |
| O | 0.32238474 | 2.42498437 | 0.00042533 |
| H | -0.72192426 | 1.90179437 | 0.00040033 |
| N | 1.59107174 | -0.96549063 | -0.00018767 |
| N | -1.54368326 | 0.85539637 | 0.00026033 |
| C | -4.90994326 | -0.76691963 | -0.00009967 |
| C | 4.90292074 | 0.83414537 | 0.00007833 |
| O | 5.40552374 | 1.93713637 | 0.00026733 |
| O | -5.46171426 | -1.84769563 | -0.00033567 |
| C | -7.02116726 | 0.32494537 | 0.00013933 |
| C | -7.55886026 | 1.74089237 | 0.00045033 |
| H | -7.33883126 | -0.23806763 | 0.88172433 |
| H | -7.33883226 | -0.23767963 | -0.88169467 |
| H | -7.22133826 | 2.28295037 | -0.88573767 |
| H | -8.65173426 | 1.72518037 | 0.00044633 |
| H | -7.22134026 | 2.28256037 | 0.88687833 |
| C | 7.05852774 | -0.16563763 | -0.00013967 |
| C | 7.65432274 | -1.55798763 | -0.00039267 |
| H | 7.35148974 | 0.40984637 | 0.88183433 |
| H | 7.35146074 | 0.41015537 | -0.88192167 |
| H | 7.33960874 | -2.11319363 | -0.88676367 |
| H | 8.74558774 | -1.49657763 | -0.00039967 |
| H | 7.33963774 | -2.11350363 | 0.88579533 |
| O | 5.61922274 | -0.31625463 | -0.00014167 |
| O | -5.57771026 | 0.41526637 | 0.00015833 |

The geometric structure coordinates of TS* of T2*-T3* path under $E_x = +1 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69586268 | 0.25067860 | -0.00058256 |
| C | 2.86650968 | -0.67632440 | -0.00082756 |
| C | 3.45966368 | 0.59017960 | -0.00216256 |
| C | 2.64077968 | 1.73126060 | -0.00275656 |
| C | 1.22813968 | 1.61368060 | -0.00205156 |
| C | -0.69424032 | -0.06618540 | 0.00041544 |
| C | -1.16090332 | -1.43452640 | 0.00169144 |
| C | -2.55354532 | -1.65078340 | 0.00250844 |
| C | -3.44628632 | -0.56746340 | 0.00211744 |
| C | -2.94685432 | 0.73736260 | 0.00091744 |
| H | 3.45723468 | -1.58130140 | -0.00037856 |
| H | 3.08310968 | 2.71863760 | -0.00384056 |
| H | -2.93199332 | -2.66413340 | 0.00346944 |
| H | -3.58834732 | 1.60565160 | 0.00058844 |
| O | -0.30433132 | -2.40506940 | 0.00204144 |
| H | 0.79601268 | -1.82963340 | 0.00109444 |
| O | 0.43284368 | 2.60578360 | -0.00262356 |
| H | -1.19622832 | 1.88997760 | -0.00090156 |
| N | 1.53326768 | -0.82269340 | -0.00006256 |
| N | -1.63023932 | 0.94671060 | 0.00016344 |
| C | -4.90435132 | -0.83111040 | 0.00302244 |
| C | 4.93063168 | 0.75576960 | -0.00299956 |
| O | 5.49495168 | 1.82670360 | -0.00420056 |
| O | -5.39248132 | -1.93807940 | 0.00407444 |
| C | -7.06963932 | 0.15022260 | 0.00334844 |
| C | -7.67626232 | 1.53755760 | 0.00289644 |
| H | -7.35585632 | -0.42723840 | 0.88595344 |
| H | -7.35675132 | -0.42819640 | -0.87834056 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.36756832 | 2.09502160 | -0.88417856 |
| H | -8.76683432 | 1.46663060 | 0.00349644 |
| H | -7.36665532 | 2.09599260 | 0.88904144 |
| C | 7.02714868 | -0.36323440 | -0.00302156 |
| C | 7.54407068 | -1.78683640 | -0.00226156 |
| H | 7.35250168 | 0.19549760 | 0.87831744 |
| H | 7.35163768 | 0.19424860 | -0.88546856 |
| H | 7.19838568 | -2.32432940 | -0.88804156 |
| H | 8.63707668 | -1.78682840 | -0.00270856 |
| H | 7.19911368 | -2.32311440 | 0.88453844 |
| O | 5.58178268 | -0.43317340 | -0.00226056 |
| O | -5.62951532 | 0.31208460 | 0.00252344 |

The geometric structure coordinates of N under $E_x = +5 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.72032800 | 0.15194100 | 0.00015200 |
| C | 2.88173100 | -0.71551000 | 0.00006100 |
| C | 3.44564400 | 0.56516900 | 0.00020400 |
| C | 2.60016300 | 1.66782200 | 0.00031800 |
| C | 1.21604500 | 1.48714800 | 0.00029500 |
| C | -0.71905400 | -0.15195300 | 0.00008100 |
| C | -1.21548700 | -1.48581700 | 0.00000700 |
| C | -2.60006200 | -1.66564100 | -0.00010700 |
| C | -3.44406600 | -0.56305200 | -0.00013700 |
| C | -2.87948700 | 0.71785500 | -0.00005100 |
| H | 3.50592100 | -1.59912300 | -0.00003500 |
| H | 3.00714000 | 2.67096500 | 0.00042900 |
| H | -3.00878400 | -2.66812900 | -0.00016300 |
| H | -3.50394700 | 1.60126100 | -0.00007300 |
| O | -0.42835000 | -2.56459700 | 0.00006400 |
| H | 0.51068000 | -2.23120100 | 0.00020800 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.42763500 | 2.56404500 | 0.00041900 |
| H | -0.51213200 | 2.22814800 | 0.00041000 |
| N | 1.56771000 | -0.90008800 | 0.00003500 |
| N | -1.56551500 | 0.90149600 | 0.00005100 |
| C | -4.91892100 | -0.79444700 | -0.00025500 |
| C | 4.91854100 | 0.79524500 | 0.00023500 |
| O | 5.43579200 | 1.88676400 | 0.00029900 |
| O | -5.42999100 | -1.88845800 | -0.00020600 |
| C | -7.05720100 | 0.23807900 | -0.00011800 |
| C | -7.62327200 | 1.64200200 | 0.00076900 |
| H | -7.35780800 | -0.33235200 | 0.88193000 |
| H | -7.35798400 | -0.33128000 | -0.88280700 |
| H | -7.29806500 | 2.19119200 | -0.88538500 |
| H | -8.71532800 | 1.60174300 | 0.00079700 |
| H | -7.29797300 | 2.19010200 | 0.88756300 |
| C | 7.05512900 | -0.23888500 | -0.00002200 |
| C | 7.62139600 | -1.64325300 | -0.00055800 |
| H | 7.35771300 | 0.33044300 | 0.88236400 |
| H | 7.35757200 | 0.33107100 | -0.88204700 |
| H | 7.29476800 | -2.19139700 | -0.88686100 |
| H | 8.71369700 | -1.60422900 | -0.00064300 |
| H | 7.29492700 | -2.19202000 | 0.88541700 |
| O | 5.61128700 | -0.36091600 | 0.00006300 |
| O | -5.61055200 | 0.35945100 | -0.00021000 |

The geometric structure coordinates of N* under $E_x = +5 \times 10^{-4}$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.69944600 | 0.15062800 | 0.00011800 |
| C | 2.87455700 | -0.70238100 | 0.00006600 |
| C | 3.45492100 | 0.58996200 | -0.00002700 |
| C | 2.60087300 | 1.70085500 | -0.00004600 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.21977300 | 1.50400100 | 0.00002800 |
| C | -0.69763500 | -0.13447600 | 0.00017900 |
| C | -1.21587000 | -1.49246300 | 0.00025900 |
| C | -2.59614000 | -1.69231000 | 0.00030500 |
| C | -3.45134100 | -0.58437700 | 0.00027700 |
| C | -2.87590500 | 0.70746700 | 0.00019500 |
| H | 3.51166600 | -1.57794800 | 0.00008500 |
| H | 3.00211400 | 2.70547500 | -0.00011000 |
| H | -2.99605400 | -2.69763600 | 0.00036200 |
| H | -3.51525200 | 1.58134400 | 0.00016800 |
| O | -0.40072700 | -2.53398500 | 0.00029100 |
| H | 0.55076300 | -2.16178200 | 0.00025500 |
| O | 0.40925000 | 2.55091100 | 0.00002800 |
| H | -0.54099400 | 2.18672200 | 0.00012800 |
| N | 1.57164400 | -0.91154300 | 0.00013600 |
| N | -1.56985900 | 0.92188400 | 0.00014900 |
| C | -4.91082700 | -0.80306200 | 0.00033100 |
| C | 4.91103900 | 0.80154400 | -0.00010000 |
| O | 5.44670400 | 1.89120300 | -0.00022800 |
| O | -5.43372600 | -1.89700800 | 0.00034400 |
| C | -7.04619300 | 0.24050900 | 0.00019900 |
| C | -7.61363200 | 1.64437900 | 0.00020600 |
| H | -7.35001200 | -0.32937200 | 0.88206100 |
| H | -7.34998900 | -0.32934700 | -0.88169000 |
| H | -7.28840900 | 2.19336700 | -0.88624700 |
| H | -8.70577600 | 1.60447800 | 0.00018500 |
| H | -7.28844200 | 2.19334200 | 0.88668700 |
| C | 7.04083500 | -0.25219400 | -0.00026300 |
| C | 7.60504100 | -1.65812900 | -0.00032700 |
| H | 7.34930900 | 0.31639700 | 0.88128600 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.34914100 | 0.31641200 | -0.88186100 |
| H | 7.27672300 | -2.20606100 | -0.88636700 |
| H | 8.69761300 | -1.62274700 | -0.00042800 |
| H | 7.27688700 | -2.20607700 | 0.88576400 |
| O | 5.60122900 | -0.36966500 | -0.00012500 |
| O | -5.60290500 | 0.36127700 | 0.00021700 |

The geometric structure coordinates of T1* under $E_x = +5 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.67353900 | 0.16661500 | 0.11803100 |
| C | 2.91412400 | -0.71972600 | 0.13826600 |
| C | 3.45095700 | 0.54153100 | -0.02946800 |
| C | 2.58515300 | 1.65773700 | -0.10672400 |
| C | 1.20641500 | 1.47689700 | -0.02652600 |
| C | -0.74563200 | -0.13124700 | 0.01758200 |
| C | -1.23593200 | -1.50761400 | -0.14952200 |
| C | -2.62704900 | -1.67303400 | -0.12511300 |
| C | -3.48545500 | -0.56345200 | -0.03835800 |
| C | -2.93136400 | 0.70703000 | 0.05465100 |
| H | 3.52052400 | -1.60849800 | 0.22342200 |
| H | 2.99121000 | 2.65451100 | -0.20380500 |
| H | -3.03671200 | -2.66437600 | -0.26407200 |
| H | -3.54729100 | 1.59568200 | 0.05627700 |
| O | -0.39798500 | -2.47229700 | -0.26057900 |
| H | 1.16508200 | -1.80974500 | 0.25019400 |
| O | 0.41160600 | 2.54643500 | -0.08337600 |
| H | -0.52343500 | 2.22899200 | 0.03397900 |
| N | 1.58395100 | -0.87251100 | 0.24810700 |
| N | -1.60473400 | 0.88299200 | 0.13148100 |
| C | -4.95109900 | -0.79064600 | -0.08622500 |
| C | 4.91433200 | 0.75719100 | -0.09176500 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.43408900 | 1.84045300 | -0.23233600 |
| O | -5.46455000 | -1.87915700 | -0.20849300 |
| C | -7.09321400 | 0.23264400 | -0.01600600 |
| C | -7.66837700 | 1.62684000 | 0.11831000 |
| H | -7.40830000 | -0.42571200 | 0.79734300 |
| H | -7.37754800 | -0.24438200 | -0.95724000 |
| H | -7.33195600 | 2.26504900 | -0.70168800 |
| H | -8.76014200 | 1.58279400 | 0.09609900 |
| H | -7.36024500 | 2.08315700 | 1.06152100 |
| C | 7.05132400 | -0.28003100 | -0.04692100 |
| C | 7.62228000 | -1.67545800 | 0.09617500 |
| H | 7.38479700 | 0.38749900 | 0.75170700 |
| H | 7.32275100 | 0.18236300 | -0.99936000 |
| H | 7.26683600 | -2.32319600 | -0.70821300 |
| H | 8.71377500 | -1.63791900 | 0.05279200 |
| H | 7.32969700 | -2.11703500 | 1.05136300 |
| O | 5.61031500 | -0.39932700 | 0.01813900 |
| O | -5.65004000 | 0.35971400 | 0.02284000 |

The geometric structure coordinates of T2* under $E_x = +5 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.74620200 | 0.14729000 | 0.02856200 |
| C | 2.93077500 | -0.69707100 | 0.06267900 |
| C | 3.49145200 | 0.57180200 | -0.02680800 |
| C | 2.63498400 | 1.68540400 | -0.10622300 |
| C | 1.24464600 | 1.52311100 | -0.12941600 |
| C | -0.67027000 | -0.14897000 | 0.12636500 |
| C | -1.20145000 | -1.46294400 | -0.01255500 |
| C | -2.57847400 | -1.64613500 | -0.09733200 |
| C | -3.44793900 | -0.53368800 | -0.02752200 |
| C | -2.91618100 | 0.72920500 | 0.13860100 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.54377200 | -1.58793100 | 0.06079200 |
| H | 3.04621500 | 2.67664700 | -0.24022000 |
| H | -2.98209200 | -2.64410500 | -0.19410400 |
| H | -3.52601400 | 1.61592800 | 0.22128800 |
| O | -0.40531300 | -2.53185900 | -0.06379800 |
| H | 0.52941200 | -2.21164900 | 0.04920100 |
| O | 0.40868800 | 2.49063500 | -0.23109400 |
| H | -1.17439400 | 1.82533000 | 0.26192300 |
| N | 1.60579400 | -0.87058400 | 0.13780400 |
| N | -1.58576500 | 0.88665900 | 0.25044200 |
| C | -4.91236500 | -0.75812000 | -0.09455000 |
| C | 4.95428100 | 0.79001900 | -0.07793600 |
| O | 5.48022900 | 1.87455700 | -0.19201200 |
| O | -5.41990300 | -1.84673700 | -0.23231900 |
| C | -7.05604100 | 0.26733000 | -0.05838300 |
| C | -7.63306800 | 1.66013100 | 0.08009400 |
| H | -7.38550000 | -0.39983100 | 0.74181800 |
| H | -7.32180600 | -0.19910800 | -1.01012200 |
| H | -7.28060800 | 2.30751700 | -0.72585600 |
| H | -8.72404400 | 1.61640000 | 0.03509600 |
| H | -7.34521800 | 2.10563400 | 1.03486200 |
| C | 7.08987700 | -0.24671800 | -0.02498300 |
| C | 7.65951800 | -1.64530900 | 0.09289200 |
| H | 7.41380400 | 0.40160300 | 0.79336900 |
| H | 7.37501100 | 0.23811300 | -0.96233600 |
| H | 7.31529400 | -2.27345600 | -0.73167300 |
| H | 8.75166200 | -1.60739600 | 0.06652800 |
| H | 7.35193300 | -2.10960600 | 1.03243000 |
| O | 5.64970300 | -0.36813400 | 0.01850700 |
| O | -5.61248300 | 0.39267500 | 0.00847400 |

The geometric structure coordinates of T3* in under $E_x = +5 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.68740600 | 0.16876300 | 0.00040400 |
| C | 2.92369100 | -0.70141000 | 0.00018200 |
| C | 3.47009800 | 0.58447900 | 0.00021500 |
| C | 2.61489900 | 1.69374700 | 0.00048900 |
| C | 1.20049700 | 1.54319400 | 0.00060000 |
| C | -0.68625500 | -0.16248800 | 0.00048800 |
| C | -1.19825100 | -1.53747100 | 0.00040600 |
| C | -2.61253500 | -1.68751500 | 0.00026400 |
| C | -3.46715800 | -0.57917700 | 0.00040300 |
| C | -2.92303000 | 0.70646600 | 0.00071500 |
| H | 3.53202200 | -1.59329800 | -0.00014200 |
| H | 3.02480300 | 2.69495400 | 0.00054500 |
| H | -3.02349400 | -2.68838500 | 0.00013000 |
| H | -3.53232100 | 1.59776100 | 0.00090200 |
| O | -0.40027000 | -2.52164300 | 0.00063900 |
| H | 1.12964100 | -1.80368600 | 0.00039100 |
| O | 0.40254100 | 2.52718700 | 0.00067700 |
| H | -1.12732300 | 1.80917400 | 0.00110900 |
| N | 1.59757500 | -0.86820700 | 0.00022300 |
| N | -1.59539300 | 0.87393000 | 0.00084300 |
| C | -4.93553900 | -0.79170500 | 0.00037400 |
| C | 4.93583200 | 0.79208500 | -0.00002400 |
| O | 5.47112100 | 1.87715000 | -0.00014200 |
| O | -5.46130100 | -1.88027900 | 0.00041300 |
| C | -7.06519600 | 0.26551200 | 0.00030900 |
| C | -7.62182200 | 1.67351300 | -0.00082400 |
| H | -7.37183000 | -0.30112900 | 0.88295300 |
| H | -7.37185900 | -0.30261200 | -0.88137400 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.29335800 | 2.21929600 | -0.88805300 |
| H | -8.71416900 | 1.64133700 | -0.00064900 |
| H | -7.29311400 | 2.22092500 | 0.88531700 |
| C | 7.06148200 | -0.27160900 | -0.00046300 |
| C | 7.61633300 | -1.68094400 | -0.00096000 |
| H | 7.37162300 | 0.29472300 | 0.88154600 |
| H | 7.37116600 | 0.29516600 | -0.88234600 |
| H | 7.28525100 | -2.22669100 | -0.88728500 |
| H | 8.70899300 | -1.65174300 | -0.00133100 |
| H | 7.28587500 | -2.22707500 | 0.88536400 |
| O | 5.61882500 | -0.38008600 | -0.00012300 |
| O | -5.61927500 | 0.37560400 | 0.00030200 |

The geometric structure coordinates of TS* of N*-T1* path under $E_x = +5 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69052149 | 0.23232580 | -0.00002768 |
| C | 2.85290549 | -0.69727220 | -0.00009268 |
| C | 3.45167949 | 0.58098180 | -0.00013268 |
| C | 2.61802549 | 1.71452180 | -0.00011768 |
| C | 1.23275249 | 1.55594480 | -0.00006568 |
| C | -0.71530051 | -0.05963520 | 0.00002732 |
| C | -1.18910151 | -1.44483620 | 0.00006432 |
| C | -2.57028951 | -1.67407820 | 0.00011832 |
| C | -3.44757851 | -0.58184720 | 0.00013432 |
| C | -2.90494351 | 0.71593780 | 0.00009532 |
| H | 3.45922349 | -1.59317820 | -0.00010268 |
| H | 3.04766549 | 2.70716880 | -0.00014668 |
| H | -2.94917251 | -2.68760720 | 0.00014632 |
| H | -3.56121251 | 1.57664480 | 0.00010632 |
| O | -0.32338951 | -2.42017020 | 0.00004732 |
| H | 0.72006849 | -1.89768220 | 0.00000232 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.44679949 | 2.63068380 | -0.00005168 |
| H | -0.49847251 | 2.30792980 | -0.00001368 |
| N | 1.54397149 | -0.85186720 | -0.00004368 |
| N | -1.58970151 | 0.96824280 | 0.00004432 |
| C | -4.90583151 | -0.83178620 | 0.00019032 |
| C | 4.91083849 | 0.76247180 | -0.00018868 |
| O | 5.47000049 | 1.84061280 | -0.00022268 |
| O | -5.40189751 | -1.93672120 | 0.00022532 |
| C | -7.06361251 | 0.16409780 | 0.00025332 |
| C | -7.65989351 | 1.55579180 | 0.00025632 |
| H | -7.35442351 | -0.41190020 | 0.88233432 |
| H | -7.35448751 | -0.41192520 | -0.88178968 |
| H | -7.34646651 | 2.11139280 | -0.88627968 |
| H | -8.75091751 | 1.49283480 | 0.00029632 |
| H | -7.34640251 | 2.11141780 | 0.88675332 |
| C | 7.01854649 | -0.33558820 | -0.00025368 |
| C | 7.55415649 | -1.75276520 | -0.00025868 |
| H | 7.33896849 | 0.22639680 | 0.88127232 |
| H | 7.33890249 | 0.22637880 | -0.88181468 |
| H | 7.21478649 | -2.29395920 | -0.88631068 |
| H | 8.64723349 | -1.73982420 | -0.00029968 |
| H | 7.21485249 | -2.29394120 | 0.88583032 |
| O | 5.57724749 | -0.42382620 | -0.00019868 |
| O | -5.62201851 | 0.31526780 | 0.00019932 |

The geometric structure coordinates of TS* of T1*-T3* path under $E_x = +5 \times 10^{-4}$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.69511884 | 0.07140556 | -0.00000874 |
| C | 2.94461184 | -0.73742944 | 0.00120326 |
| C | 3.44757384 | 0.56702356 | -0.00038574 |
| C | 2.55633384 | 1.65258556 | -0.00182074 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.16316284 | 1.43821456 | -0.00167574 |
| C | -0.69712016 | -0.24436244 | 0.00025226 |
| C | -1.22770316 | -1.60769444 | 0.00189826 |
| C | -2.64000016 | -1.72505844 | 0.00191226 |
| C | -3.45846016 | -0.58406244 | 0.00041426 |
| C | -2.86723316 | 0.68191656 | -0.00110574 |
| H | 3.58391184 | -1.60726844 | 0.00234926 |
| H | 2.93615484 | 2.66536356 | -0.00305074 |
| H | -3.08338416 | -2.71203344 | 0.00309526 |
| H | -3.45807016 | 1.58675356 | -0.00229074 |
| O | -0.43101516 | -2.59924044 | 0.00320526 |
| H | 1.18955684 | -1.88568744 | 0.00248026 |
| O | 0.30733184 | 2.40956756 | -0.00296674 |
| H | -0.79204316 | 1.83608756 | -0.00234874 |
| N | 1.62857884 | -0.94346044 | 0.00134626 |
| N | -1.53201016 | 0.82820356 | -0.00115974 |
| C | -4.93138616 | -0.75300944 | 0.00048026 |
| C | 4.90446484 | 0.82550056 | -0.00057874 |
| O | 5.40019384 | 1.92987356 | -0.00190574 |
| O | -5.48955116 | -1.82637344 | 0.00175726 |
| C | -7.03070916 | 0.36132656 | -0.00111274 |
| C | -7.54914916 | 1.78398856 | -0.00290074 |
| H | -7.35351016 | -0.19637044 | 0.88157426 |
| H | -7.35333416 | -0.19852444 | -0.88250074 |
| H | -7.20522416 | 2.32032856 | -0.89003374 |
| H | -8.64201216 | 1.78179656 | -0.00300874 |
| H | -7.20540316 | 2.32249156 | 0.88299026 |
| C | 7.06592684 | -0.16329744 | 0.00083526 |
| C | 7.66939784 | -1.55240244 | 0.00257226 |
| H | 7.35546784 | 0.41483356 | 0.88215726 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.35561584 | 0.41269256 | -0.88183874 |
| H | 7.35810484 | -2.11059444 | -0.88316874 |
| H | 8.76033484 | -1.48496544 | 0.00258126 |
| H | 7.35795784 | -2.10844344 | 0.88961226 |
| O | 5.62752584 | -0.32188644 | 0.00090726 |
| O | -5.58332816 | 0.43266956 | -0.00105674 |

The geometric structure coordinates of TS* of N*-T2* path under $E_x = +5 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.71296688 | 0.06751093 | -0.00003025 |
| C | 2.90073388 | -0.71371407 | -0.00008325 |
| C | 3.44725188 | 0.58681493 | -0.00016325 |
| C | 2.57041888 | 1.68033993 | -0.00017725 |
| C | 1.18870788 | 1.45157293 | -0.00011025 |
| C | -0.68721912 | -0.22293107 | 0.00003875 |
| C | -1.22970512 | -1.54986507 | 0.00011875 |
| C | -2.61420412 | -1.70920507 | 0.00018075 |
| C | -3.44756812 | -0.57751207 | 0.00016375 |
| C | -2.85284712 | 0.70083293 | 0.00008275 |
| H | 3.55796788 | -1.57390007 | -0.00007125 |
| H | 2.94886088 | 2.69387593 | -0.00023725 |
| H | -3.04407212 | -2.70191907 | 0.00024175 |
| H | -3.46172712 | 1.59504893 | 0.00006675 |
| O | -0.44106812 | -2.62136307 | 0.00013575 |
| H | 0.50467188 | -2.29413407 | 0.00008275 |
| O | 0.32419388 | 2.42769293 | -0.00011925 |
| H | -0.72101212 | 1.90546393 | -0.00005425 |
| N | 1.59094388 | -0.96537907 | -0.00001925 |
| N | -1.54242612 | 0.85939993 | 0.00002475 |
| C | -4.91026812 | -0.76445507 | 0.00022875 |
| C | 4.90198888 | 0.83032493 | -0.00023225 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.41015288 | 1.93149093 | -0.00030125 |
| O | -5.45826712 | -1.84642407 | 0.00029975 |
| C | -7.02269512 | 0.32553793 | 0.00026275 |
| C | -7.56035112 | 1.74120993 | 0.00021975 |
| H | -7.33908912 | -0.23747307 | 0.88212775 |
| H | -7.33915812 | -0.23755207 | -0.88152725 |
| H | -7.22353212 | 2.28314593 | -0.88628525 |
| H | -8.65311412 | 1.72475393 | 0.00026275 |
| H | -7.22346212 | 2.28322693 | 0.88664875 |
| C | 7.05506488 | -0.17448307 | -0.00027425 |
| C | 7.64899688 | -1.56792907 | -0.00023625 |
| H | 7.35010188 | 0.40062093 | 0.88144275 |
| H | 7.35003088 | 0.40054193 | -0.88206725 |
| H | 7.33282988 | -2.12280907 | -0.88632325 |
| H | 8.74049388 | -1.50875707 | -0.00028325 |
| H | 7.33290188 | -2.12273007 | 0.88592675 |
| O | 5.61712088 | -0.32314707 | -0.00021025 |
| O | -5.57768712 | 0.41575893 | 0.00020175 |

The geometric structure coordinates of TS* of T2*-T3* path under $E_x = +5 \times 10^{-4}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69542983 | 0.25389672 | 0.00111320 |
| C | 2.86499883 | -0.67670028 | -0.00206380 |
| C | 3.46130883 | 0.58932972 | 0.00273520 |
| C | 2.64374183 | 1.73160172 | 0.00688820 |
| C | 1.23069683 | 1.61584072 | 0.00626220 |
| C | -0.69381317 | -0.06171828 | -0.00025280 |
| C | -1.16143017 | -1.43037828 | -0.00546380 |
| C | -2.55402617 | -1.64589228 | -0.00651080 |
| C | -3.44625617 | -0.56284528 | -0.00260080 |
| C | -2.94722917 | 0.74154972 | 0.00238620 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.45436283 | -1.58260328 | -0.00537280 |
| H | 3.08677083 | 2.71861572 | 0.01061620 |
| H | -2.93302317 | -2.65907528 | -0.01036980 |
| H | -3.58889417 | 1.60974872 | 0.00554420 |
| O | -0.30564817 | -2.40153528 | -0.00895980 |
| H | 0.79577983 | -1.82641028 | -0.00663780 |
| O | 0.43767783 | 2.60941972 | 0.00985820 |
| H | -1.19771017 | 1.89445672 | 0.00699620 |
| N | 1.53287783 | -0.82120828 | -0.00277480 |
| N | -1.62993417 | 0.95111972 | 0.00340520 |
| C | -4.90544317 | -0.82789328 | -0.00384180 |
| C | 4.93118083 | 0.75060972 | 0.00351120 |
| O | 5.50112283 | 1.81913372 | 0.00755020 |
| O | -5.39009317 | -1.93590828 | -0.00805280 |
| C | -7.07189517 | 0.15157172 | -0.00057780 |
| C | -7.67868617 | 1.53856072 | 0.00437320 |
| H | -7.35757617 | -0.42976728 | 0.87950120 |
| H | -7.35725117 | -0.42332628 | -0.88498280 |
| H | -7.37007717 | 2.09986572 | -0.88028480 |
| H | -8.76911717 | 1.46682572 | 0.00390820 |
| H | -7.37040917 | 2.09339372 | 0.89321920 |
| C | 7.02426283 | -0.37446928 | -0.00043580 |
| C | 7.53821883 | -1.79939528 | -0.00559080 |
| H | 7.35133683 | 0.17951172 | 0.88343220 |
| H | 7.35153383 | 0.18596372 | -0.88015280 |
| H | 7.19127883 | -2.33220328 | -0.89372680 |
| H | 8.63132283 | -1.80233628 | -0.00548280 |
| H | 7.19108483 | -2.33868328 | 0.87854920 |
| O | 5.58014083 | -0.44147228 | -0.00084480 |
| O | -5.63039317 | 0.31358872 | 0.00027920 |

The geometric structure coordinates of N under $E_x = +1 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.72098400 | 0.15196700 | -0.00008700 |
| C | 2.88290300 | -0.71430500 | -0.00006700 |
| C | 3.44650800 | 0.56626800 | 0.00009200 |
| C | 2.60026300 | 1.66897000 | 0.00013700 |
| C | 1.21637900 | 1.48787300 | 0.00002900 |
| C | -0.71834000 | -0.15186400 | -0.00009600 |
| C | -1.21520000 | -1.48506100 | -0.00026200 |
| C | -2.60000600 | -1.66443000 | -0.00029200 |
| C | -3.44326500 | -0.56185600 | -0.00013300 |
| C | -2.87828300 | 0.71917700 | 0.00006700 |
| H | 3.50697200 | -1.59802200 | -0.00011700 |
| H | 3.00637100 | 2.67244000 | 0.00022700 |
| H | -3.00962600 | -2.66658100 | -0.00042000 |
| H | -3.50287100 | 1.60248600 | 0.00020900 |
| O | -0.42870400 | -2.56476700 | -0.00036500 |
| H | 0.50996500 | -2.23257500 | -0.00024800 |
| O | 0.42730800 | 2.56378200 | -0.00001000 |
| H | -0.51285400 | 2.22659700 | -0.00024300 |
| N | 1.56887200 | -0.89936000 | -0.00015000 |
| N | -1.56434600 | 0.90233600 | 0.00008600 |
| C | -4.91908900 | -0.79392700 | -0.00015600 |
| C | 4.91841300 | 0.79565300 | 0.00018900 |
| O | 5.43883300 | 1.88588200 | 0.00030500 |
| O | -5.42698500 | -1.88922300 | -0.00027500 |
| C | -7.05834000 | 0.23762000 | 0.00007500 |
| C | -7.62446900 | 1.64125600 | 0.00101800 |
| H | -7.35796100 | -0.33301100 | 0.88218400 |
| H | -7.35813100 | -0.33186700 | -0.88272300 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.29999200 | 2.19061100 | -0.88528900 |
| H | -8.71640300 | 1.60025000 | 0.00105100 |
| H | -7.29989200 | 2.18945200 | 0.88800600 |
| C | 7.05414300 | -0.23936900 | 0.00017000 |
| C | 7.62049400 | -1.64396800 | -0.00022900 |
| H | 7.35758500 | 0.32987700 | 0.88247100 |
| H | 7.35760900 | 0.33039900 | -0.88178300 |
| H | 7.29331000 | -2.19207000 | -0.88636400 |
| H | 8.71293200 | -1.60555500 | -0.00020900 |
| H | 7.29329500 | -2.19258800 | 0.88557900 |
| O | 5.61170400 | -0.36170000 | 0.00012300 |
| O | -5.61024900 | 0.35880300 | -0.00000700 |

The geometric structure coordinates of N* under $E_x = +1 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.70089800 | 0.15906300 | 0.00022200 |
| C | 2.87414400 | -0.69982900 | -0.00006800 |
| C | 3.45719300 | 0.59258800 | 0.00035200 |
| C | 2.60378700 | 1.70492600 | 0.00073900 |
| C | 1.22211000 | 1.50976700 | 0.00069800 |
| C | -0.69728600 | -0.12636100 | 0.00004700 |
| C | -1.21418500 | -1.48638300 | -0.00047000 |
| C | -2.59418300 | -1.68769100 | -0.00060300 |
| C | -3.45000600 | -0.58131800 | -0.00025500 |
| C | -2.87693900 | 0.71014000 | 0.00020700 |
| H | 3.50975500 | -1.57648900 | -0.00039000 |
| H | 3.00580700 | 2.70916500 | 0.00107900 |
| H | -2.99348700 | -2.69336400 | -0.00097100 |
| H | -3.51711700 | 1.58336100 | 0.00046900 |
| O | -0.39688200 | -2.52537600 | -0.00082900 |
| H | 0.55523500 | -2.14938600 | -0.00074200 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.41420200 | 2.55969200 | 0.00112900 |
| H | -0.53540600 | 2.19991600 | 0.00113800 |
| N | 1.57244500 | -0.90577700 | -0.00014900 |
| N | -1.56898100 | 0.92678200 | 0.00034200 |
| C | -4.91124100 | -0.80376000 | -0.00039600 |
| C | 4.91174800 | 0.80068400 | 0.00038700 |
| O | 5.45381100 | 1.88818300 | 0.00075600 |
| O | -5.42766300 | -1.89989700 | -0.00072700 |
| C | -7.04952600 | 0.23452800 | 0.00003600 |
| C | -7.61885900 | 1.63725200 | 0.00067700 |
| H | -7.35093900 | -0.33641900 | 0.88181800 |
| H | -7.35099100 | -0.33563000 | -0.88224000 |
| H | -7.29531700 | 2.18720100 | -0.88575800 |
| H | -8.71079100 | 1.59486100 | 0.00068500 |
| H | -7.29527300 | 2.18640700 | 0.88758800 |
| C | 7.03877000 | -0.25815200 | -0.00001900 |
| C | 7.60152300 | -1.66505400 | -0.00056000 |
| H | 7.34945400 | 0.30950300 | 0.88161300 |
| H | 7.34941100 | 0.31016600 | -0.88123900 |
| H | 7.27183000 | -2.21217400 | -0.88662900 |
| H | 8.69431300 | -1.63179400 | -0.00057000 |
| H | 7.27186800 | -2.21284000 | 0.88511200 |
| O | 5.60100700 | -0.37406100 | -0.00002700 |
| O | -5.60440000 | 0.35716800 | 0.00004400 |

The geometric structure coordinates of T1* under $E_x = +1 \times 10^{-3}$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.67489700 | 0.17433700 | -0.11307100 |
| C | 2.91358100 | -0.71494400 | -0.13864700 |
| C | 3.45260900 | 0.54508200 | 0.03293600 |
| C | 2.58788300 | 1.66262800 | 0.11615400 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.20873700 | 1.48303500 | 0.03740000 |
| C | -0.74513800 | -0.12452900 | -0.01304300 |
| C | -1.23263300 | -1.50179600 | 0.15120700 |
| C | -2.62382600 | -1.66818600 | 0.12573500 |
| C | -3.48294600 | -0.55988800 | 0.04047500 |
| C | -2.93161700 | 0.71170800 | -0.04839700 |
| H | 3.51825700 | -1.60454900 | -0.22691600 |
| H | 2.99483100 | 2.65868000 | 0.21616100 |
| H | -3.03311900 | -2.66008300 | 0.26210600 |
| H | -3.54877700 | 1.59943300 | -0.04806400 |
| O | -0.39349800 | -2.46587700 | 0.26086400 |
| H | 1.16176400 | -1.80202600 | -0.25114000 |
| O | 0.41438400 | 2.55259900 | 0.09939900 |
| H | -0.52089900 | 2.23656100 | -0.01950100 |
| N | 1.58350800 | -0.86536700 | -0.24787900 |
| N | -1.60452500 | 0.88845100 | -0.12457600 |
| C | -4.94988100 | -0.79131600 | 0.08572100 |
| C | 4.91518900 | 0.75688400 | 0.09407700 |
| O | 5.44054400 | 1.83732000 | 0.23895400 |
| O | -5.45753600 | -1.88219800 | 0.20696100 |
| C | -7.09496900 | 0.22612800 | 0.01096600 |
| C | -7.67257800 | 1.61879400 | -0.12543700 |
| H | -7.37927600 | -0.25113700 | 0.95192300 |
| H | -7.40562900 | -0.43349400 | -0.80286100 |
| H | -7.36391700 | 2.07527100 | -1.06837500 |
| H | -8.76416000 | 1.57178700 | -0.10566300 |
| H | -7.34009200 | 2.25827800 | 0.69515000 |
| C | 7.04930900 | -0.28524400 | 0.04361900 |
| C | 7.61795700 | -1.68130500 | -0.10530200 |
| H | 7.32287600 | 0.17262100 | 0.99780500 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.38492500 | 0.38478900 | -0.75221700 |
| H | 7.32374500 | -2.11842500 | -1.06205800 |
| H | 8.70967000 | -1.64646200 | -0.06205300 |
| H | 7.26090700 | -2.33158300 | 0.69633800 |
| O | 5.60966100 | -0.40200100 | -0.02160000 |
| O | -5.65029400 | 0.35591000 | -0.02465600 |

The geometric structure coordinates of T2* under $E_x = +1 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.74626300 | 0.15697500 | 0.03600400 |
| C | 2.93033000 | -0.69050500 | 0.06535800 |
| C | 3.49453500 | 0.57804100 | -0.01865700 |
| C | 2.63882800 | 1.69371200 | -0.09034600 |
| C | 1.24870200 | 1.53302100 | -0.11198500 |
| C | -0.66842800 | -0.13940600 | 0.13119000 |
| C | -1.19796200 | -1.45579500 | -0.00638600 |
| C | -2.57393200 | -1.64051300 | -0.09464000 |
| C | -3.44614800 | -0.53087000 | -0.02765000 |
| C | -2.91740700 | 0.73314500 | 0.13881200 |
| H | 3.54201500 | -1.58236700 | 0.05877300 |
| H | 3.05047800 | 2.68548200 | -0.21858400 |
| H | -2.97577200 | -2.63923800 | -0.19244000 |
| H | -3.52955400 | 1.61838100 | 0.22102700 |
| O | -0.40044800 | -2.52359800 | -0.05478000 |
| H | 0.53420300 | -2.20095200 | 0.05527800 |
| O | 0.41372200 | 2.50228500 | -0.20335200 |
| H | -1.17960600 | 1.83303900 | 0.26913000 |
| N | 1.60644000 | -0.86328400 | 0.13933700 |
| N | -1.58729000 | 0.89345200 | 0.25170800 |
| C | -4.91080100 | -0.76060700 | -0.09740200 |
| C | 4.95569900 | 0.79169500 | -0.07139700 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.48812600 | 1.87445600 | -0.17849000 |
| O | -5.41151800 | -1.85205900 | -0.23511300 |
| C | -7.05848800 | 0.25758700 | -0.06458400 |
| C | -7.63948500 | 1.64851900 | 0.07309600 |
| H | -7.38564000 | -0.41051200 | 0.73559100 |
| H | -7.32095700 | -0.20994300 | -1.01654900 |
| H | -7.28885700 | 2.29688600 | -0.73284800 |
| H | -8.73016000 | 1.60099500 | 0.02708900 |
| H | -7.35446400 | 2.09507000 | 1.02820500 |
| C | 7.08795000 | -0.25210000 | -0.03125700 |
| C | 7.65488100 | -1.65315400 | 0.07372500 |
| H | 7.41673800 | 0.38857800 | 0.79140100 |
| H | 7.37314400 | 0.23954200 | -0.96523300 |
| H | 7.30643100 | -2.27364100 | -0.75488100 |
| H | 8.74719600 | -1.61818200 | 0.04488800 |
| H | 7.34797500 | -2.12439300 | 1.01005200 |
| O | 5.64935100 | -0.37084300 | 0.01485500 |
| O | -5.61372900 | 0.38680900 | 0.00355000 |

The geometric structure coordinates of T3* in under $E_x = +1 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.68805300 | 0.17187300 | 0.00018500 |
| C | 2.92406300 | -0.69889800 | -0.00021900 |
| C | 3.47167200 | 0.58712600 | 0.00035600 |
| C | 2.61614900 | 1.69682100 | 0.00085100 |
| C | 1.20168000 | 1.54601800 | 0.00075900 |
| C | -0.68571400 | -0.15943400 | 0.00004200 |
| C | -1.19712300 | -1.53464000 | -0.00050300 |
| C | -2.61149800 | -1.68431800 | -0.00055500 |
| C | -3.46577800 | -0.57649900 | -0.00006300 |
| C | -2.92260600 | 0.70910900 | 0.00046700 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.53184900 | -1.59113100 | -0.00058200 |
| H | 3.02554600 | 2.69818800 | 0.00133600 |
| H | -3.02296800 | -2.68503200 | -0.00100400 |
| H | -3.53235300 | 1.60012200 | 0.00082000 |
| O | -0.39917700 | -2.51885600 | -0.00093600 |
| H | 1.13065500 | -1.80072500 | -0.00068500 |
| O | 0.40369300 | 2.52986900 | 0.00119100 |
| H | -1.12624400 | 1.81201500 | 0.00093200 |
| N | 1.59866800 | -0.86527900 | -0.00027000 |
| N | -1.59429700 | 0.87669100 | 0.00049800 |
| C | -4.93550000 | -0.79138300 | -0.00016400 |
| C | 4.93608800 | 0.79229400 | 0.00048700 |
| O | 5.47606300 | 1.87570900 | 0.00096200 |
| O | -5.45662500 | -1.88168600 | -0.00056000 |
| C | -7.06712200 | 0.26245800 | 0.00019100 |
| C | -7.62477500 | 1.66972600 | 0.00029800 |
| H | -7.37200700 | -0.30548300 | 0.88242300 |
| H | -7.37199500 | -0.30530300 | -0.88215900 |
| H | -7.29731700 | 2.21676000 | -0.88651900 |
| H | -8.71696800 | 1.63588600 | 0.00020300 |
| H | -7.29744100 | 2.21663900 | 0.88722800 |
| C | 7.05981900 | -0.27467300 | 0.00003200 |
| C | 7.61375400 | -1.68466600 | -0.00073600 |
| H | 7.37137100 | 0.29097300 | 0.88218200 |
| H | 7.37131800 | 0.29197400 | -0.88149400 |
| H | 7.28182900 | -2.22982400 | -0.88712800 |
| H | 8.70658200 | -1.65695900 | -0.00079700 |
| H | 7.28196900 | -2.23071400 | 0.88516900 |
| O | 5.61871300 | -0.38232400 | 0.00001600 |
| O | -5.61957800 | 0.37357400 | 0.00023500 |

The geometric structure coordinates of TS* of N*-T1* path under $E_x = +1 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69194058 | 0.23873809 | -0.01305923 |
| C | 2.85456958 | -0.68898191 | 0.01227577 |
| C | 3.45271158 | 0.58936509 | -0.04099123 |
| C | 2.61642658 | 1.72121209 | -0.08120823 |
| C | 1.23104858 | 1.56057109 | -0.06780323 |
| C | -0.71671142 | -0.05686491 | 0.00574777 |
| C | -1.18599542 | -1.44234991 | 0.06267477 |
| C | -2.56648842 | -1.67465991 | 0.07893477 |
| C | -3.44666442 | -0.58582391 | 0.04068677 |
| C | -2.90902442 | 0.71067409 | -0.01317923 |
| H | 3.46121158 | -1.58404291 | 0.04433977 |
| H | 3.04384858 | 2.71389209 | -0.12240823 |
| H | -2.94321242 | -2.68821991 | 0.12067377 |
| H | -3.56666942 | 1.56967209 | -0.04371923 |
| O | -0.31734742 | -2.41458091 | 0.09648977 |
| H | 0.72451658 | -1.88965991 | 0.07036577 |
| O | 0.44421358 | 2.63468109 | -0.10600723 |
| H | -0.50009542 | 2.31280409 | -0.08850323 |
| N | 1.54651858 | -0.84353691 | 0.02507177 |
| N | -1.59137842 | 0.96573509 | -0.02999823 |
| C | -4.90603242 | -0.84214791 | 0.05833177 |
| C | 4.90971158 | 0.77093809 | -0.05549423 |
| O | 5.47212458 | 1.84748809 | -0.10038923 |
| O | -5.39323142 | -1.94929891 | 0.10418677 |
| C | -7.06868742 | 0.14348509 | 0.03123877 |
| C | -7.66983842 | 1.53180709 | -0.01887023 |
| H | -7.35120042 | -0.39939191 | 0.93650377 |
| H | -7.36068542 | -0.46713791 | -0.82661923 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.36440742 | 2.05398109 | -0.92818723 |
| H | -8.76044542 | 1.46432109 | -0.00990323 |
| H | -7.35406042 | 2.12233909 | 0.84389877 |
| C | 7.01739658 | -0.32632491 | -0.02349023 |
| C | 7.55505958 | -1.74213191 | 0.02864577 |
| H | 7.34311658 | 0.26949809 | 0.83378277 |
| H | 7.33398658 | 0.20115509 | -0.92767223 |
| H | 7.21110158 | -2.31749891 | -0.83382323 |
| H | 8.64825758 | -1.72878591 | 0.02247377 |
| H | 7.22024058 | -2.24885991 | 0.93657277 |
| O | 5.57814958 | -0.41632191 | -0.01252723 |
| O | -5.62565342 | 0.29925409 | 0.01747877 |

The geometric structure coordinates of TS* of T1*-T3* path under $E_x = +1 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.70230309 | 0.10639166 | -0.07436620 |
| C | 2.91619209 | -0.75022934 | 0.19866480 |
| C | 3.47120209 | 0.49435266 | -0.11722120 |
| C | 2.62326509 | 1.57335366 | -0.41914020 |
| C | 1.22287609 | 1.41188966 | -0.40594020 |
| C | -0.70217091 | -0.15525434 | -0.03961220 |
| C | -1.28236191 | -1.45739334 | 0.28729980 |
| C | -2.69756291 | -1.52694234 | 0.27343480 |
| C | -3.47182591 | -0.39862234 | -0.04021720 |
| C | -2.83460191 | 0.80705866 | -0.34103220 |
| H | 3.51987509 | -1.61224234 | 0.43892280 |
| H | 3.04234109 | 2.53998966 | -0.66389020 |
| H | -3.17847591 | -2.46753234 | 0.50753380 |
| H | -3.39112691 | 1.69976466 | -0.58788820 |
| O | -0.52278691 | -2.44040634 | 0.56206580 |
| H | 1.11550609 | -1.80149934 | 0.43543580 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.40537309 | 2.37860566 | -0.67660920 |
| H | -0.71454291 | 1.85972066 | -0.56598220 |
| N | 1.59407509 | -0.90503934 | 0.21159780 |
| N | -1.49386291 | 0.90717266 | -0.33542620 |
| C | -4.95118591 | -0.51879334 | -0.04428420 |
| C | 4.93540809 | 0.69437466 | -0.13837620 |
| O | 5.47877309 | 1.74399066 | -0.40304720 |
| O | -5.54149091 | -1.54354334 | 0.21113780 |
| C | -7.00830991 | 0.64196866 | -0.38856320 |
| C | -7.57803791 | 0.79737366 | 1.01144880 |
| H | -7.34839791 | -0.28454434 | -0.85405120 |
| H | -7.26611991 | 1.48652466 | -1.02740020 |
| H | -7.19269291 | 1.70299266 | 1.48563080 |
| H | -8.66780791 | 0.87056866 | 0.96165480 |
| H | -7.31822691 | -0.06608434 | 1.62504880 |
| C | 7.05386909 | -0.33543334 | 0.17797180 |
| C | 7.60114109 | -1.69710834 | 0.55349280 |
| H | 7.34910309 | 0.43946066 | 0.89036380 |
| H | 7.38612809 | -0.01565134 | -0.81327120 |
| H | 7.28413709 | -2.45347434 | -0.16795320 |
| H | 8.69384509 | -1.66954434 | 0.56791180 |
| H | 7.24994709 | -1.99522334 | 1.54386080 |
| O | 5.61227709 | -0.44077234 | 0.17468380 |
| O | -5.55553291 | 0.64641566 | -0.36802820 |

The geometric structure coordinates of TS* of N*-T2* path under $E_x = +1 \times 10^{-3}$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.71198721 | 0.07201022 | 0.01102986 |
| C | 2.90021821 | -0.70715178 | -0.02663314 |
| C | 3.44615221 | 0.59183922 | 0.07425186 |
| C | 2.56736321 | 1.68186722 | 0.14662086 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.18577421 | 1.45213922 | 0.11714186 |
| C | -0.68545479 | -0.21878978 | -0.02284114 |
| C | -1.22549279 | -1.54421878 | -0.12550014 |
| C | -2.60934879 | -1.70502578 | -0.14973714 |
| C | -3.44461879 | -0.57838178 | -0.07390114 |
| C | -2.85412579 | 0.69718522 | 0.02557686 |
| H | 3.55941921 | -1.56401178 | -0.08394514 |
| H | 2.94356921 | 2.69316322 | 0.22460586 |
| H | -3.03753979 | -2.69557578 | -0.22665414 |
| H | -3.46564479 | 1.58755922 | 0.08600386 |
| O | -0.43370979 | -2.61042678 | -0.19714314 |
| H | 0.51158921 | -2.28102478 | -0.16429014 |
| O | 0.32000121 | 2.42490222 | 0.18105786 |
| H | -0.72524379 | 1.90260222 | 0.13330886 |
| N | 1.59342021 | -0.95927078 | -0.05715914 |
| N | -1.54314879 | 0.85843022 | 0.04906786 |
| C | -4.90869179 | -0.76929178 | -0.10079114 |
| C | 4.89862121 | 0.83348022 | 0.10530586 |
| O | 5.41058821 | 1.93053022 | 0.19056286 |
| O | -5.44914979 | -1.85085778 | -0.18582014 |
| C | -7.02537179 | 0.31133022 | -0.03854414 |
| C | -7.56662179 | 1.72173722 | 0.06133086 |
| H | -7.34627379 | -0.31623078 | 0.79667086 |
| H | -7.33134379 | -0.18595878 | -0.96238714 |
| H | -7.22457279 | 2.32851422 | -0.77997714 |
| H | -8.65916479 | 1.70224622 | 0.05067786 |
| H | -7.23949279 | 2.19754422 | 0.98845786 |
| C | 7.05130421 | -0.17031078 | 0.05143386 |
| C | 7.64688221 | -1.56011078 | -0.04470914 |
| H | 7.33907721 | 0.33882622 | 0.97534386 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.35537721 | 0.46746222 | -0.78309514 |
| H | 7.33873321 | -2.04891178 | -0.97163614 |
| H | 8.73846021 | -1.50148878 | -0.03033314 |
| H | 7.32240721 | -2.17812778 | 0.79543386 |
| O | 5.61551821 | -0.31925378 | 0.02723686 |
| O | -5.57871279 | 0.40399322 | -0.01937514 |

The geometric structure coordinates of TS* of T2*-T3* path under $E_x = +1 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.70336400 | 0.27817506 | 0.13301560 |
| C | 2.83560300 | -0.68141994 | -0.19632040 |
| C | 3.48146500 | 0.51368106 | 0.14483060 |
| C | 2.70793700 | 1.63355106 | 0.49310560 |
| C | 1.29142100 | 1.56634406 | 0.50241160 |
| C | -0.69510300 | 0.01746606 | 0.08619060 |
| C | -1.21355100 | -1.28067594 | -0.28834740 |
| C | -2.61281000 | -1.44515994 | -0.30834540 |
| C | -3.46411500 | -0.38175894 | 0.02600260 |
| C | -2.91797100 | 0.85301606 | 0.38141260 |
| H | 3.38961000 | -1.56777994 | -0.47119140 |
| H | 3.18743400 | 2.56606806 | 0.75935260 |
| H | -3.02910600 | -2.40471894 | -0.58444340 |
| H | -3.52769700 | 1.70345306 | 0.64682460 |
| O | -0.39507000 | -2.23712494 | -0.58913540 |
| H | 0.72851900 | -1.71829494 | -0.45910040 |
| O | 0.53824600 | 2.54344806 | 0.80782960 |
| H | -1.12928100 | 1.90679606 | 0.65587460 |
| N | 1.50087400 | -0.77857994 | -0.19706440 |
| N | -1.59347400 | 1.01520406 | 0.40151760 |
| C | -4.93301700 | -0.59420894 | -0.00498440 |
| C | 4.95443000 | 0.62001406 | 0.14603760 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.56970300 | 1.62418106 | 0.43122960 |
| O | -5.45066500 | -1.64450194 | -0.30788740 |
| C | -7.06393700 | 0.42681306 | 0.33773960 |
| C | -7.61621500 | 0.59684306 | -1.06728240 |
| H | -7.38326900 | 1.23103806 | 1.00018160 |
| H | -7.35371700 | -0.53462094 | 0.76464960 |
| H | -7.29267900 | -0.22649894 | -1.70527940 |
| H | -8.70907200 | 0.60076306 | -1.03654340 |
| H | -7.28017800 | 1.54102606 | -1.50201540 |
| C | 7.00004100 | -0.52717894 | -0.23579240 |
| C | 7.45750000 | -1.90941394 | -0.65490840 |
| H | 7.36727100 | -0.25463894 | 0.75735960 |
| H | 7.33294500 | 0.24651306 | -0.93296640 |
| H | 7.07126900 | -2.16014994 | -1.64536940 |
| H | 8.54952000 | -1.94800394 | -0.68918240 |
| H | 7.10676700 | -2.66351794 | 0.05317960 |
| O | 5.55635700 | -0.54513894 | -0.21175240 |
| O | -5.61254000 | 0.51952406 | 0.34629560 |

The geometric structure coordinates of N under $E_x = +2 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.72230300 | 0.15223100 | 0.00006100 |
| C | 2.88526400 | -0.71183600 | -0.00006700 |
| C | 3.44836000 | 0.56851800 | 0.00008100 |
| C | 2.60061400 | 1.67139000 | 0.00023400 |
| C | 1.21718800 | 1.48956200 | 0.00023200 |
| C | -0.71679400 | -0.15140700 | 0.00001700 |
| C | -1.21459600 | -1.48332600 | -0.00015200 |
| C | -2.59986100 | -1.66181600 | -0.00016100 |
| C | -3.44169700 | -0.55927700 | -0.00001600 |
| C | -2.87584400 | 0.72204500 | 0.00013300 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.50909100 | -1.59577500 | -0.00018500 |
| H | 3.00512800 | 2.67546200 | 0.00036000 |
| H | -3.01121800 | -2.66331500 | -0.00028600 |
| H | -3.50070800 | 1.60515700 | 0.00024500 |
| O | -0.42935100 | -2.56480500 | -0.00031500 |
| H | 0.50866900 | -2.23493300 | -0.00031400 |
| O | 0.42686900 | 2.56351000 | 0.00040200 |
| H | -0.51417400 | 2.22384100 | 0.00040600 |
| N | 1.57122100 | -0.89777200 | -0.00007600 |
| N | -1.56201300 | 0.90429600 | 0.00014800 |
| C | -4.91939200 | -0.79269800 | -0.00002900 |
| C | 4.91828700 | 0.79649700 | 0.00008600 |
| O | 5.44504300 | 1.88409900 | 0.00024700 |
| O | -5.42092200 | -1.89060400 | -0.00018600 |
| C | -7.06086000 | 0.23648000 | 0.00001800 |
| C | -7.62736900 | 1.63942200 | 0.00072500 |
| H | -7.35837900 | -0.33443400 | 0.88237000 |
| H | -7.35841800 | -0.33353900 | -0.88290500 |
| H | -7.30439900 | 2.18897100 | -0.88599000 |
| H | -8.71907500 | 1.59673300 | 0.00069200 |
| H | -7.30441300 | 2.18806500 | 0.88800600 |
| C | 7.05226900 | -0.24061700 | 0.00001100 |
| C | 7.61873700 | -1.64570800 | -0.00034100 |
| H | 7.35771800 | 0.32836400 | 0.88212500 |
| H | 7.35771000 | 0.32881000 | -0.88181500 |
| H | 7.29029000 | -2.19365700 | -0.88612600 |
| H | 8.71146800 | -1.60847600 | -0.00033800 |
| H | 7.29030200 | -2.19410100 | 0.88517400 |
| O | 5.61260400 | -0.36337700 | -0.00000900 |
| O | -5.60981200 | 0.35762500 | 0.00003100 |

The geometric structure coordinates of N* under $E_x = +2 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.70493400 | 0.17763100 | 0.00024900 |
| C | 2.87398400 | -0.69402800 | 0.00015300 |
| C | 3.46281800 | 0.59798100 | 0.00036300 |
| C | 2.61077800 | 1.71342700 | 0.00052000 |
| C | 1.22774100 | 1.52203600 | 0.00046900 |
| C | -0.69762200 | -0.10869200 | 0.00016500 |
| C | -1.21087100 | -1.47277600 | -0.00002700 |
| C | -2.59053300 | -1.67796200 | -0.00011300 |
| C | -3.44822600 | -0.57498800 | -0.00001600 |
| C | -2.88028300 | 0.71540900 | 0.00016500 |
| H | 3.50546900 | -1.57362000 | 0.00002800 |
| H | 3.01457200 | 2.71679500 | 0.00068700 |
| H | -2.98796000 | -2.68456800 | -0.00025400 |
| H | -3.52177200 | 1.58753600 | 0.00024500 |
| O | -0.38853900 | -2.50588800 | -0.00012500 |
| H | 0.56551800 | -2.12074000 | -0.00004000 |
| O | 0.42561700 | 2.57885300 | 0.00063900 |
| H | -0.52235000 | 2.22926400 | 0.00060800 |
| N | 1.57393700 | -0.89209900 | 0.00010100 |
| N | -1.56750400 | 0.93675800 | 0.00025000 |
| C | -4.91283400 | -0.80559200 | -0.00010700 |
| C | 4.91417000 | 0.79889500 | 0.00042000 |
| O | 5.46921800 | 1.88209200 | 0.00039500 |
| O | -5.41557000 | -1.90645300 | -0.00020400 |
| C | -7.05736900 | 0.22155400 | 0.00007600 |
| C | -7.63098300 | 1.62176500 | 0.00031400 |
| H | -7.35383400 | -0.35059700 | 0.88234300 |
| H | -7.35386300 | -0.35030800 | -0.88236800 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.31098700 | 2.17273900 | -0.88669800 |
| H | -8.72248300 | 1.57392700 | 0.00032200 |
| H | -7.31096100 | 2.17244900 | 0.88749800 |
| C | 7.03528100 | -0.27128800 | -0.00022800 |
| C | 7.59457700 | -1.68034800 | -0.00069700 |
| H | 7.35094000 | 0.29509000 | 0.88100100 |
| H | 7.35062800 | 0.29555200 | -0.88127100 |
| H | 7.26171200 | -2.22648000 | -0.88627000 |
| H | 8.68783800 | -1.65171800 | -0.00088100 |
| H | 7.26202400 | -2.22694500 | 0.88470800 |
| O | 5.60112500 | -0.38349800 | 0.00000000 |
| O | -5.60849700 | 0.34844100 | 0.00007200 |

The geometric structure coordinates of T1* under $E_x = +2 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.67745900 | 0.18705700 | 0.10747300 |
| C | 2.91207700 | -0.70820200 | 0.13469900 |
| C | 3.45598100 | 0.55129600 | -0.03172000 |
| C | 2.59308300 | 1.67188100 | -0.11659400 |
| C | 1.21314400 | 1.49429700 | -0.04238900 |
| C | -0.74422400 | -0.11283700 | 0.00573500 |
| C | -1.22636400 | -1.49058100 | -0.16122100 |
| C | -2.61835500 | -1.65796700 | -0.13821700 |
| C | -3.47832100 | -0.55234500 | -0.05031900 |
| C | -2.93155200 | 0.72069800 | 0.03990200 |
| H | 3.51327100 | -1.60035100 | 0.22054400 |
| H | 3.00171900 | 2.66752800 | -0.21282500 |
| H | -3.02701300 | -2.64992600 | -0.27678500 |
| H | -3.55061800 | 1.60696100 | 0.04070100 |
| O | -0.38578600 | -2.45344900 | -0.27114500 |
| H | 1.15424200 | -1.79024900 | 0.23662900 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.41947600 | 2.56410000 | -0.10397800 |
| H | -0.51651800 | 2.24916100 | 0.01405500 |
| N | 1.58249000 | -0.85473300 | 0.24019500 |
| N | -1.60360300 | 0.89784500 | 0.11797500 |
| C | -4.94784500 | -0.79053100 | -0.09470300 |
| C | 4.91675600 | 0.75610500 | -0.08764700 |
| O | 5.45338900 | 1.83228300 | -0.23078100 |
| O | -5.44471300 | -1.88468100 | -0.22355300 |
| C | -7.09815000 | 0.21664100 | -0.00804700 |
| C | -7.67974700 | 1.60565100 | 0.14159300 |
| H | -7.40229700 | -0.45124300 | 0.80111100 |
| H | -7.38074800 | -0.25385300 | -0.95260700 |
| H | -7.35291700 | 2.25344600 | -0.67469000 |
| H | -8.77096000 | 1.55374100 | 0.12400500 |
| H | -7.37166500 | 2.05520000 | 1.08799800 |
| C | 7.04523100 | -0.29618600 | -0.03375300 |
| C | 7.60941200 | -1.69471800 | 0.11464600 |
| H | 7.38453800 | 0.37173200 | 0.76274300 |
| H | 7.32366000 | 0.16122200 | -0.98712000 |
| H | 7.24988700 | -2.34289800 | -0.68762400 |
| H | 8.70159500 | -1.66465700 | 0.07278400 |
| H | 7.31136900 | -2.13159900 | 1.07036200 |
| O | 5.60827100 | -0.40865300 | 0.02978800 |
| O | -5.65040000 | 0.35038200 | 0.02526700 |

The geometric structure coordinates of T2* under $E_x = +2 \times 10^{-3}$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.74672900 | 0.17476100 | 0.04511200 |
| C | 2.92904900 | -0.68004600 | 0.07447500 |
| C | 3.50126000 | 0.58661700 | -0.01178700 |
| C | 2.64772800 | 1.70620700 | -0.08003400 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.25803700 | 1.54903200 | -0.09763600 |
| C | -0.66517000 | -0.11970600 | 0.13843700 |
| C | -1.19318100 | -1.44116900 | 0.01844300 |
| C | -2.56756700 | -1.62856700 | -0.07131500 |
| C | -3.44343000 | -0.52263600 | -0.02061600 |
| C | -2.91893100 | 0.74462700 | 0.13126100 |
| H | 3.53762600 | -1.57428000 | 0.06837800 |
| H | 3.06113800 | 2.69728900 | -0.20698000 |
| H | -2.96722000 | -2.62933400 | -0.15917900 |
| H | -3.53396800 | 1.62887400 | 0.20299000 |
| O | -0.39446900 | -2.50856400 | -0.01509900 |
| H | 0.54020000 | -2.18187900 | 0.08508800 |
| O | 0.42561700 | 2.52155400 | -0.17947600 |
| H | -1.18658100 | 1.85108200 | 0.25948600 |
| N | 1.60727700 | -0.84971300 | 0.14752800 |
| N | -1.58866400 | 0.91000700 | 0.24231300 |
| C | -4.90913600 | -0.76193700 | -0.09085800 |
| C | 4.95920200 | 0.78993700 | -0.06938500 |
| O | 5.50524200 | 1.86766700 | -0.17388400 |
| O | -5.39758300 | -1.85984900 | -0.21543500 |
| C | -7.06352800 | 0.24470200 | -0.07248200 |
| C | -7.65046100 | 1.63403300 | 0.04909000 |
| H | -7.38561200 | -0.41593400 | 0.73554300 |
| H | -7.32139000 | -0.23518200 | -1.01924300 |
| H | -7.30394900 | 2.27491300 | -0.76455000 |
| H | -8.74065600 | 1.57975500 | 0.00330400 |
| H | -7.36914800 | 2.09287700 | 0.99942000 |
| C | 7.08419300 | -0.26859900 | -0.04246400 |
| C | 7.64495300 | -1.67352600 | 0.05248700 |
| H | 7.42247400 | 0.36559600 | 0.78186800 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.37040700 | 0.22622600 | -0.97486200 |
| H | 7.28834200 | -2.28758800 | -0.77748500 |
| H | 8.73762900 | -1.64520400 | 0.01895700 |
| H | 7.33858600 | -2.14817400 | 0.98732700 |
| O | 5.64866300 | -0.38086600 | 0.00925200 |
| O | -5.61599000 | 0.38058000 | -0.00549800 |

The geometric structure coordinates of T3* in under $E_x = +2 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.68943000 | 0.17810600 | -0.00049100 |
| C | 2.92460600 | -0.69387900 | -0.00068800 |
| C | 3.47502800 | 0.59254500 | -0.00016900 |
| C | 2.61869900 | 1.70284200 | 0.00016500 |
| C | 1.20399300 | 1.55157700 | 0.00007800 |
| C | -0.68490400 | -0.15327500 | -0.00065400 |
| C | -1.19502500 | -1.52882800 | -0.00113800 |
| C | -2.60950800 | -1.67789800 | -0.00078700 |
| C | -3.46328200 | -0.57123800 | -0.00033300 |
| C | -2.92183200 | 0.71433200 | -0.00006300 |
| H | 3.53118100 | -1.58687800 | -0.00100000 |
| H | 3.02701200 | 2.70458900 | 0.00054700 |
| H | -3.02202900 | -2.67830800 | -0.00098300 |
| H | -3.53237600 | 1.60487000 | 0.00025000 |
| O | -0.39703500 | -2.51314100 | -0.00179400 |
| H | 1.13267300 | -1.79474500 | -0.00123700 |
| O | 0.40600100 | 2.53518700 | 0.00046300 |
| H | -1.12399300 | 1.81744800 | 0.00016600 |
| N | 1.60074700 | -0.85917600 | -0.00083600 |
| N | -1.59216300 | 0.88209700 | -0.00019400 |
| C | -4.93554900 | -0.79096600 | -0.00009600 |
| C | 4.93666800 | 0.79291600 | 0.00003600 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.48621200 | 1.87300000 | 0.00053900 |
| O | -5.44735500 | -1.88475800 | -0.00021400 |
| C | -7.07118300 | 0.25641000 | 0.00073900 |
| C | -7.63101700 | 1.66218600 | 0.00130000 |
| H | -7.37233500 | -0.31258000 | 0.88323900 |
| H | -7.37298600 | -0.31212500 | -0.88182900 |
| H | -7.30596800 | 2.21027200 | -0.88571000 |
| H | -8.72291800 | 1.62495100 | 0.00116700 |
| H | -7.30613900 | 2.20958500 | 0.88879500 |
| C | 7.05651900 | -0.28094900 | -0.00010200 |
| C | 7.60889400 | -1.69220200 | 0.00090400 |
| H | 7.37117600 | 0.28498300 | 0.88119100 |
| H | 7.37163100 | 0.28377000 | -0.88204200 |
| H | 7.27514500 | -2.23774000 | -0.88462600 |
| H | 8.70207600 | -1.66731000 | 0.00107900 |
| H | 7.27480000 | -2.23663500 | 0.88697600 |
| O | 5.61863200 | -0.38700000 | -0.00043300 |
| O | -5.62039000 | 0.36950400 | 0.00027300 |

The geometric structure coordinates of TS* of N*-T1* path under $E_x = +2 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69686918 | 0.24774495 | 0.00004841 |
| C | 2.85342918 | -0.69221205 | -0.00018159 |
| C | 3.45944518 | 0.58536195 | 0.00008841 |
| C | 2.62567618 | 1.72144395 | 0.00034441 |
| C | 1.23883018 | 1.56554395 | 0.00032741 |
| C | -0.72071682 | -0.04725405 | 0.00000141 |
| C | -1.18996082 | -1.43299605 | -0.00029159 |
| C | -2.57092882 | -1.66348605 | -0.00032659 |
| C | -3.44967082 | -0.57338005 | -0.00008259 |
| C | -2.91303882 | 0.72015295 | 0.00019241 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.45388618 | -1.59186105 | -0.00038459 |
| H | 3.05573118 | 2.71374695 | 0.00055441 |
| H | -2.95027682 | -2.67710105 | -0.00054159 |
| H | -3.56728282 | 1.58203295 | 0.00038541 |
| O | -0.32194782 | -2.40660105 | -0.00051159 |
| H | 0.72136218 | -1.88079105 | -0.00041159 |
| O | 0.45781818 | 2.64599995 | 0.00057041 |
| H | -0.48684282 | 2.33137295 | 0.00051341 |
| N | 1.54550218 | -0.83782805 | -0.00019759 |
| N | -1.58841682 | 0.97271095 | 0.00023241 |
| C | -4.91297982 | -0.83410005 | -0.00012359 |
| C | 4.91354118 | 0.75875395 | 0.00010741 |
| O | 5.48965918 | 1.83125095 | 0.00033441 |
| O | -5.39011382 | -1.94520005 | -0.00035759 |
| C | -7.07878282 | 0.14691295 | 0.00010841 |
| C | -7.68015282 | 1.53530795 | 0.00040841 |
| H | -7.36287882 | -0.43097305 | 0.88253041 |
| H | -7.36289482 | -0.43059805 | -0.88255259 |
| H | -7.37142782 | 2.09261095 | -0.88660259 |
| H | -8.77044382 | 1.46538195 | 0.00040341 |
| H | -7.37141082 | 2.09223495 | 0.88764941 |
| C | 7.01389618 | -0.35243805 | -0.00016359 |
| C | 7.54640518 | -1.77188505 | -0.00048059 |
| H | 7.34035818 | 0.20769995 | 0.88109141 |
| H | 7.34033318 | 0.20808395 | -0.88118259 |
| H | 7.20342018 | -2.31168005 | -0.88609759 |
| H | 8.64000918 | -1.76415905 | -0.00049459 |
| H | 7.20344518 | -2.31206605 | 0.88491041 |
| O | 5.57802218 | -0.43743305 | -0.00016259 |
| O | -5.63177082 | 0.30330295 | 0.00012841 |

The geometric structure coordinates of TS* of T1*-T3* path under $E_x = +2 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69754992 | 0.08595497 | -0.00040957 |
| C | 2.94009592 | -0.73206003 | 0.00491743 |
| C | 3.45031692 | 0.57261897 | -0.00369457 |
| C | 2.56050392 | 1.66161497 | -0.01082957 |
| C | 1.16625292 | 1.45008097 | -0.00938957 |
| C | -0.70004208 | -0.22999703 | 0.00159743 |
| C | -1.22335008 | -1.59459803 | 0.01048543 |
| C | -2.63477308 | -1.71445203 | 0.01122743 |
| C | -3.45471908 | -0.57558803 | 0.00375843 |
| C | -2.87046008 | 0.69051997 | -0.00448757 |
| H | 3.57487492 | -1.60499703 | 0.01066043 |
| H | 2.94204692 | 2.67364397 | -0.01748057 |
| H | -3.07875408 | -2.70134303 | 0.01763143 |
| H | -3.46326908 | 1.59388997 | -0.01043057 |
| O | -0.42102908 | -2.58310303 | 0.01696743 |
| H | 1.17526592 | -1.87167703 | 0.01243543 |
| O | 0.31045792 | 2.42156997 | -0.01574357 |
| H | -0.78731708 | 1.84986097 | -0.01199557 |
| N | 1.62569292 | -0.93116603 | 0.00628343 |
| N | -1.53077108 | 0.83875397 | -0.00539557 |
| C | -4.93200908 | -0.75600703 | 0.00484743 |
| C | 4.90345992 | 0.82128597 | -0.00536757 |
| O | 5.41627492 | 1.92026197 | -0.01257557 |
| O | -5.47255908 | -1.83666703 | 0.01184343 |
| C | -7.04080508 | 0.34238897 | -0.00244157 |
| C | -7.56635308 | 1.76144697 | -0.01154757 |
| H | -7.35682208 | -0.21310803 | 0.88352043 |
| H | -7.35670408 | -0.22439003 | -0.88127257 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.22751008 | 2.29533097 | -0.90204157 |
| H | -8.65887308 | 1.75118397 | -0.01155957 |
| H | -7.22763608 | 2.30666497 | 0.87210043 |
| C | 7.05723792 | -0.18247703 | 0.00110843 |
| C | 7.65579992 | -1.57469903 | 0.01001743 |
| H | 7.35323292 | 0.39860597 | 0.87900843 |
| H | 7.35313892 | 0.38728197 | -0.88421257 |
| H | 7.34007392 | -2.13605303 | -0.87223557 |
| H | 8.74753392 | -1.51365703 | 0.00956443 |
| H | 7.34017392 | -2.12468103 | 0.89943943 |
| O | 5.62350792 | -0.33578403 | 0.00216943 |
| O | -5.58846708 | 0.42049397 | -0.00284957 |

The geometric structure coordinates of TS* of N*-T2* path under $E_x = +2 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.71117832 | 0.07815086 | 0.00000484 |
| C | 2.89615432 | -0.71099214 | -0.00017316 |
| C | 3.44836532 | 0.59341986 | 0.00005784 |
| C | 2.57146332 | 1.68825386 | 0.00027184 |
| C | 1.18844532 | 1.45954686 | 0.00025084 |
| C | -0.68392668 | -0.21078814 | -0.00002716 |
| C | -1.22672168 | -1.54141914 | -0.00026316 |
| C | -2.61057668 | -1.70088014 | -0.00027216 |
| C | -3.44313368 | -0.57191114 | -0.00005316 |
| C | -2.85312368 | 0.70614886 | 0.00017184 |
| H | 3.55416832 | -1.57084614 | -0.00034116 |
| H | 2.94879032 | 2.70201186 | 0.00045184 |
| H | -3.04140668 | -2.69347314 | -0.00044816 |
| H | -3.46420468 | 1.59887186 | 0.00034384 |
| O | -0.43509568 | -2.60919614 | -0.00046916 |
| H | 0.51121232 | -2.27705114 | -0.00042316 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.32554932 | 2.43670386 | 0.00044384 |
| H | -0.72316268 | 1.91351286 | 0.00036384 |
| N | 1.59316532 | -0.96097114 | -0.00019916 |
| N | -1.53967168 | 0.86805386 | 0.00018184 |
| C | -4.91119668 | -0.76664314 | -0.00006816 |
| C | 4.89789032 | 0.82866886 | 0.00007884 |
| O | 5.42322432 | 1.92480686 | 0.00027284 |
| O | -5.44300768 | -1.85427714 | -0.00025916 |
| C | -7.03037368 | 0.31243986 | 0.00016084 |
| C | -7.57103468 | 1.72587886 | 0.00042384 |
| H | -7.34103068 | -0.25233714 | 0.88232684 |
| H | -7.34105768 | -0.25201914 | -0.88220016 |
| H | -7.23798268 | 2.26918886 | -0.88656816 |
| H | -8.66338668 | 1.70413886 | 0.00043684 |
| H | -7.23795668 | 2.26886886 | 0.88760284 |
| C | 7.04481032 | -0.18819214 | -0.00014216 |
| C | 7.63668132 | -1.58364914 | -0.00040516 |
| H | 7.34557432 | 0.38556886 | 0.88127684 |
| H | 7.34554632 | 0.38588786 | -0.88136216 |
| H | 7.31720432 | -2.13749614 | -0.88606716 |
| H | 8.72888132 | -1.52893014 | -0.00041316 |
| H | 7.31723332 | -2.13781714 | 0.88506584 |
| O | 5.61234432 | -0.33439914 | -0.00014516 |
| O | -5.57969868 | 0.40533286 | 0.00015684 |

The geometric structure coordinates of TS* of T2*-T3* path under $E_x = +2 \times 10^{-3}$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.69315597 | 0.26828517 | 0.00082379 |
| C | 2.86179997 | -0.66868283 | -0.00203321 |
| C | 3.46598297 | 0.59783717 | 0.00170279 |
| C | 2.64913297 | 1.74142717 | 0.00512979 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.23470897 | 1.62764917 | 0.00483879 |
| C | -0.69248503 | -0.04777483 | -0.00006821 |
| C | -1.15883203 | -1.41928183 | -0.00414621 |
| C | -2.55081803 | -1.63617483 | -0.00477321 |
| C | -3.44478103 | -0.55729483 | -0.00154921 |
| C | -2.95097703 | 0.74733017 | 0.00233579 |
| H | 3.44886797 | -1.57623683 | -0.00475521 |
| H | 3.09132197 | 2.72868917 | 0.00803879 |
| H | -2.92869403 | -2.64998983 | -0.00778321 |
| H | -3.59572303 | 1.61340317 | 0.00492879 |
| O | -0.30284903 | -2.38968183 | -0.00704921 |
| H | 0.80290697 | -1.81079883 | -0.00535421 |
| O | 0.44693397 | 2.62419217 | 0.00782279 |
| H | -1.20893003 | 1.90639117 | 0.00575879 |
| N | 1.53439097 | -0.81008183 | -0.00240121 |
| N | -1.63176003 | 0.96128717 | 0.00296179 |
| C | -4.90716603 | -0.83243583 | -0.00234721 |
| C | 4.93105697 | 0.74825517 | 0.00207979 |
| O | 5.51838297 | 1.80988317 | 0.00519979 |
| O | -5.37523903 | -1.94604483 | -0.00562921 |
| C | -7.08125803 | 0.13323317 | 0.00051779 |
| C | -7.69341803 | 1.51688117 | 0.00451879 |
| H | -7.36057703 | -0.44907283 | 0.88147279 |
| H | -7.36057803 | -0.44396983 | -0.88378821 |
| H | -7.38960103 | 2.07902617 | -0.88118721 |
| H | -8.78310203 | 1.43833617 | 0.00428979 |
| H | -7.38960503 | 2.07389717 | 0.89346079 |
| C | 7.01523197 | -0.39252683 | -0.00142421 |
| C | 7.52339497 | -1.82051983 | -0.00563621 |
| H | 7.34893597 | 0.15990517 | 0.88162879 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.34883197 | 0.16506717 | -0.88126621 |
| H | 7.17193897 | -2.35213983 | -0.89278421 |
| H | 8.61689497 | -1.83039783 | -0.00573221 |
| H | 7.17204797 | -2.35732383 | 0.87842779 |
| O | 5.57601697 | -0.45379383 | -0.00152121 |
| O | -5.63506603 | 0.30065317 | 0.00100179 |

The geometric structure coordinates of N under $E_x = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.72355200 | 0.15250200 | 0.00003100 |
| C | 2.88756300 | -0.70942800 | 0.00012100 |
| C | 3.45025900 | 0.57074000 | 0.00028300 |
| C | 2.60098300 | 1.67384600 | 0.00029200 |
| C | 1.21803100 | 1.49127300 | 0.00015300 |
| C | -0.71513100 | -0.15071700 | -0.00004400 |
| C | -1.21392900 | -1.48142100 | -0.00018900 |
| C | -2.59965100 | -1.65899500 | -0.00029100 |
| C | -3.44011300 | -0.55646400 | -0.00022800 |
| C | -2.87327600 | 0.72520400 | -0.00004900 |
| H | 3.51113900 | -1.59361300 | 0.00010000 |
| H | 3.00391800 | 2.67851600 | 0.00038800 |
| H | -3.01277800 | -2.65983000 | -0.00040600 |
| H | -3.49846300 | 1.60810100 | 0.00001400 |
| O | -0.42979800 | -2.56450200 | -0.00020700 |
| H | 0.50761500 | -2.23679500 | -0.00005200 |
| O | 0.42631700 | 2.56308800 | 0.00010400 |
| H | -0.51556300 | 2.22061000 | -0.00011200 |
| N | 1.57355700 | -0.89626600 | 0.00000500 |
| N | -1.55957400 | 0.90657500 | 0.00003900 |
| C | -4.91965100 | -0.79126900 | -0.00034400 |
| C | 4.91817800 | 0.79726300 | 0.00042600 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.45130400 | 1.88222300 | 0.00037100 |
| O | -5.41478800 | -1.89177500 | -0.00030700 |
| C | -7.06351600 | 0.23527200 | 0.00010400 |
| C | -7.63072300 | 1.63739200 | 0.00089100 |
| H | -7.35863200 | -0.33611900 | 0.88268600 |
| H | -7.35890500 | -0.33522300 | -0.88297100 |
| H | -7.30961800 | 2.18733500 | -0.88623700 |
| H | -8.72219900 | 1.59270600 | 0.00101400 |
| H | -7.30938000 | 2.18643000 | 0.88849500 |
| C | 7.05057200 | -0.24201500 | 0.00003000 |
| C | 7.61716400 | -1.64759400 | -0.00041800 |
| H | 7.35809000 | 0.32664600 | 0.88197800 |
| H | 7.35788800 | 0.32713100 | -0.88167400 |
| H | 7.28740800 | -2.19534300 | -0.88586100 |
| H | 8.71023200 | -1.61151500 | -0.00053100 |
| H | 7.28760900 | -2.19582900 | 0.88479900 |
| O | 5.61360000 | -0.36520000 | 0.00016600 |
| O | -5.60945200 | 0.35666200 | -0.00007500 |

The geometric structure coordinates of N* under $E_x = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.71053000 | 0.19594300 | 0.00009600 |
| C | 2.87470300 | -0.68862900 | -0.00005800 |
| C | 3.46983500 | 0.60224500 | 0.00016000 |
| C | 2.61913500 | 1.72063500 | 0.00036500 |
| C | 1.23466600 | 1.53366800 | 0.00034400 |
| C | -0.69941200 | -0.09156900 | 0.00003700 |
| C | -1.20883600 | -1.45864500 | -0.00022100 |
| C | -2.58838300 | -1.66763400 | -0.00024700 |
| C | -3.44811200 | -0.56780400 | -0.00004000 |
| C | -2.88474800 | 0.72084300 | 0.00018600 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.50091200 | -1.57187600 | -0.00021600 |
| H | 3.02513000 | 2.72300000 | 0.00054600 |
| H | -2.98384600 | -2.67521400 | -0.00043300 |
| H | -3.52659800 | 1.59254700 | 0.00035200 |
| O | -0.38199400 | -2.48666200 | -0.00044600 |
| H | 0.57364400 | -2.09361100 | -0.00044700 |
| O | 0.43876800 | 2.59798400 | 0.00057300 |
| H | -0.50744100 | 2.25957600 | 0.00056800 |
| N | 1.57518500 | -0.87741200 | -0.00008900 |
| N | -1.56601400 | 0.94582100 | 0.00022300 |
| C | -4.91602700 | -0.80664200 | -0.00007400 |
| C | 4.91819500 | 0.79647000 | 0.00018300 |
| O | 5.48601900 | 1.87562300 | 0.00035100 |
| O | -5.40497400 | -1.91231800 | -0.00024000 |
| C | -7.06722000 | 0.20872500 | 0.00020600 |
| C | -7.64582200 | 1.60610400 | 0.00051100 |
| H | -7.35840500 | -0.36503800 | 0.88280100 |
| H | -7.35847200 | -0.36468100 | -0.88260000 |
| H | -7.32975100 | 2.15853800 | -0.88692600 |
| H | -8.73688000 | 1.55221200 | 0.00054100 |
| H | -7.32968500 | 2.15817800 | 0.88814800 |
| C | 7.03391500 | -0.28413800 | -0.00008500 |
| C | 7.59059400 | -1.69500700 | -0.00037500 |
| H | 7.35386900 | 0.28111300 | 0.88088400 |
| H | 7.35381600 | 0.28145500 | -0.88085400 |
| H | 7.25520300 | -2.24029400 | -0.88559600 |
| H | 8.68433700 | -1.67033800 | -0.00040300 |
| H | 7.25525600 | -2.24063700 | 0.88465500 |
| O | 5.60326800 | -0.39346800 | -0.00006300 |
| O | -5.61452400 | 0.34053700 | 0.00017600 |

The geometric structure coordinates of T1* under $E_x = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.67957600 | 0.19592100 | -0.10261500 |
| C | 2.91148400 | -0.70268100 | -0.12733100 |
| C | 3.45960500 | 0.55676700 | 0.03408400 |
| C | 2.59628400 | 1.67916300 | 0.11978700 |
| C | 1.21659400 | 1.50316300 | 0.04789600 |
| C | -0.74291900 | -0.10528300 | -0.00325100 |
| C | -1.22201900 | -1.48458900 | 0.15317600 |
| C | -2.61473000 | -1.65127400 | 0.13344400 |
| C | -3.47468800 | -0.54688800 | 0.05188900 |
| C | -2.93108200 | 0.72800500 | -0.03020400 |
| H | 3.50951900 | -1.59723100 | -0.20980700 |
| H | 3.00551700 | 2.67476700 | 0.21368300 |
| H | -3.02352200 | -2.64409100 | 0.26590300 |
| H | -3.55127100 | 1.61337600 | -0.02570300 |
| O | -0.38047900 | -2.44806600 | 0.25126100 |
| H | 1.14861000 | -1.78071500 | -0.22592800 |
| O | 0.42250100 | 2.57239900 | 0.10817600 |
| H | -0.51415600 | 2.25743300 | -0.00689400 |
| N | 1.58281100 | -0.84593600 | -0.22985800 |
| N | -1.60274500 | 0.90432000 | -0.10817500 |
| C | -4.94685700 | -0.79039000 | 0.09480700 |
| C | 4.91767800 | 0.75650900 | 0.08645300 |
| O | 5.46440000 | 1.82908000 | 0.22899400 |
| O | -5.43413500 | -1.88802500 | 0.22475600 |
| C | -7.10142100 | 0.20943500 | 0.00474400 |
| C | -7.68574200 | 1.59635400 | -0.14768900 |
| H | -7.38194200 | -0.26070500 | 0.94981000 |
| H | -7.40046100 | -0.46060100 | -0.80419100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.37874400 | 2.04540200 | -1.09464000 |
| H | -8.77663000 | 1.54043100 | -0.13157000 |
| H | -7.36322100 | 2.24629400 | 0.66855800 |
| C | 7.04189600 | -0.30359900 | 0.03128200 |
| C | 7.60375100 | -1.70373000 | -0.11682000 |
| H | 7.32353900 | 0.15307500 | 0.98446400 |
| H | 7.38509700 | 0.36314500 | -0.76502000 |
| H | 7.30365400 | -2.14014600 | -1.07214900 |
| H | 8.69633500 | -1.67698400 | -0.07499800 |
| H | 7.24169700 | -2.35084000 | 0.68522300 |
| O | 5.60791100 | -0.41365600 | -0.03241900 |
| O | -5.65041400 | 0.34591100 | -0.02663300 |

The geometric structure coordinates of T2* under $E_x = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.74728400 | 0.19188400 | -0.05286800 |
| C | 2.92736600 | -0.66894800 | -0.08046600 |
| C | 3.50761200 | 0.59705300 | 0.00397400 |
| C | 2.65572500 | 1.71964800 | 0.06568000 |
| C | 1.26517500 | 1.56494400 | 0.07966200 |
| C | -0.66237600 | -0.10249100 | -0.14272400 |
| C | -1.18829700 | -1.42823100 | -0.03791400 |
| C | -2.56180800 | -1.61803700 | 0.05344500 |
| C | -3.44066300 | -0.51635100 | 0.01679600 |
| C | -2.91953500 | 0.75426500 | -0.12144500 |
| H | 3.53383100 | -1.56487100 | -0.07228800 |
| H | 3.06968700 | 2.71098300 | 0.18833100 |
| H | -2.95951700 | -2.62062800 | 0.13222300 |
| H | -3.53738400 | 1.63743300 | -0.18356800 |
| O | -0.38860700 | -2.49482600 | -0.01794900 |
| H | 0.54633400 | -2.16414400 | -0.10870400 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.43659500 | 2.54105400 | 0.14849800 |
| H | -1.18977900 | 1.86621500 | -0.24323000 |
| N | 1.60772900 | -0.83772400 | -0.15168600 |
| N | -1.58957800 | 0.92398300 | -0.23007100 |
| C | -4.90764600 | -0.76468300 | 0.08661500 |
| C | 4.96220600 | 0.79044000 | 0.06455600 |
| O | 5.52191300 | 1.86351600 | 0.16311900 |
| O | -5.38405400 | -1.86849900 | 0.19980100 |
| C | -7.06843500 | 0.23106000 | 0.07962700 |
| C | -7.66077200 | 1.61852100 | -0.02920400 |
| H | -7.32211300 | -0.25893300 | 1.02204700 |
| H | -7.38525100 | -0.42372300 | -0.73487800 |
| H | -7.38267500 | 2.08741300 | -0.97552200 |
| H | -8.75051700 | 1.55783900 | 0.01585800 |
| H | -7.31864800 | 2.25350600 | 0.79084800 |
| C | 7.08011400 | -0.28254300 | 0.05068900 |
| C | 7.63522400 | -1.69119300 | -0.03185100 |
| H | 7.36854900 | 0.21764600 | 0.97999800 |
| H | 7.42657300 | 0.34340400 | -0.77710200 |
| H | 7.32835100 | -2.17147700 | -0.96370800 |
| H | 8.72828400 | -1.66887800 | 0.00486500 |
| H | 7.27196100 | -2.29710900 | 0.80127300 |
| O | 5.64770300 | -0.38907200 | -0.00442200 |
| O | -5.61786100 | 0.37290400 | 0.01418700 |

The geometric structure coordinates of T3* in under $E_x = +3 \times 10^{-3}$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.69424200 | 0.22050600 | 0.00017700 |
| C | 2.92154200 | -0.67258900 | -0.00032600 |
| C | 3.48824000 | 0.60853100 | -0.00018600 |
| C | 2.64059300 | 1.72632000 | 0.00015600 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.22323200 | 1.58921400 | 0.00039000 |
| C | -0.68101400 | -0.11250800 | 0.00020700 |
| C | -1.18046300 | -1.49258200 | 0.00006700 |
| C | -2.59351200 | -1.65451900 | 0.00035800 |
| C | -3.45750000 | -0.55830600 | 0.00065000 |
| C | -2.92961100 | 0.73193300 | 0.00066700 |
| H | 3.51773100 | -1.57259700 | -0.00053900 |
| H | 3.05635200 | 2.72498100 | 0.00031600 |
| H | -2.99663400 | -2.65888600 | 0.00029700 |
| H | -3.54879000 | 1.61652300 | 0.00080700 |
| O | -0.37661200 | -2.47291300 | -0.00026700 |
| H | 1.11398000 | -1.75704700 | -0.00028900 |
| O | 0.43864800 | 2.58144300 | 0.00079500 |
| H | -1.16078900 | 1.85227100 | 0.00060400 |
| N | 1.59768800 | -0.82396100 | -0.00014000 |
| N | -1.60027800 | 0.91209700 | 0.00043700 |
| C | -4.93026400 | -0.79661800 | 0.00089200 |
| C | 4.94855300 | 0.79044600 | -0.00036000 |
| O | 5.51814500 | 1.86198300 | -0.00019600 |
| O | -5.42220400 | -1.89862000 | 0.00083100 |
| C | -7.07962500 | 0.22496800 | 0.00132200 |
| C | -7.65437200 | 1.62405500 | 0.00091400 |
| H | -7.37233900 | -0.34709900 | 0.88434500 |
| H | -7.37250600 | -0.34767800 | -0.88126100 |
| H | -7.33703400 | 2.17518600 | -0.88695300 |
| H | -8.74558900 | 1.57343600 | 0.00100800 |
| H | -7.33690600 | 2.17576900 | 0.88837000 |
| C | 7.05421500 | -0.31055800 | -0.00085000 |
| C | 7.59194200 | -1.72814100 | -0.00137400 |
| H | 7.37800800 | 0.25066900 | 0.88067000 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.37774100 | 0.25121900 | -0.88211400 |
| H | 7.25071900 | -2.26911400 | -0.88690500 |
| H | 8.68567700 | -1.71624100 | -0.00160500 |
| H | 7.25109500 | -2.26964700 | 0.88397600 |
| O | 5.61877300 | -0.40162900 | -0.00066300 |
| O | -5.62637900 | 0.35309700 | 0.00114500 |

The geometric structure coordinates of TS* of N*-T1* path under $E_x = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.70227317 | 0.25619175 | -0.00459952 |
| C | 2.85212817 | -0.69734325 | 0.01049348 |
| C | 3.46696417 | 0.57747775 | -0.01296052 |
| C | 2.63646017 | 1.71703875 | -0.03261252 |
| C | 1.24800617 | 1.56821775 | -0.02864152 |
| C | -0.72578683 | -0.03719425 | 0.00131248 |
| C | -1.19446983 | -1.42097725 | 0.02532448 |
| C | -2.57636883 | -1.64837225 | 0.03030848 |
| C | -3.45345183 | -0.55712525 | 0.01222848 |
| C | -2.91741283 | 0.73187975 | -0.01048652 |
| H | 3.44458217 | -1.60188325 | 0.02622648 |
| H | 3.07017817 | 2.70755875 | -0.05069152 |
| H | -2.95903583 | -2.66076725 | 0.04779248 |
| H | -3.56758683 | 1.59644075 | -0.02511152 |
| O | -0.32706583 | -2.39495925 | 0.04122548 |
| H | 0.72150817 | -1.86612025 | 0.03254148 |
| O | 0.47363817 | 2.65462575 | -0.04739152 |
| H | -0.47168183 | 2.34843075 | -0.04086852 |
| N | 1.54336717 | -0.83103525 | 0.01421548 |
| N | -1.58528483 | 0.98028875 | -0.01565652 |
| C | -4.92060183 | -0.82142525 | 0.01771448 |
| C | 4.91848717 | 0.74190375 | -0.01709952 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.50864517 | 1.80906675 | -0.03681352 |
| O | -5.38789983 | -1.93541425 | 0.03634848 |
| C | -7.08965283 | 0.15499575 | 0.00331248 |
| C | -7.69121983 | 1.54235675 | -0.02109652 |
| H | -7.37016283 | -0.40724425 | 0.89653348 |
| H | -7.37127683 | -0.43881725 | -0.86892952 |
| H | -7.38466283 | 2.08392875 | -0.91847452 |
| H | -8.78121983 | 1.47029475 | -0.01949152 |
| H | -7.38413583 | 2.11539875 | 0.85633948 |
| C | 7.01071917 | -0.38421425 | 0.00157948 |
| C | 7.53715117 | -1.80639125 | 0.02881048 |
| H | 7.34337117 | 0.19109975 | 0.87121348 |
| H | 7.34217317 | 0.15684775 | -0.89023852 |
| H | 7.18965117 | -2.36171325 | -0.84543952 |
| H | 8.63114717 | -1.80516125 | 0.02795148 |
| H | 7.19099617 | -2.32729025 | 0.92451848 |
| O | 5.57808417 | -0.46283325 | 0.00406748 |
| O | -5.63863483 | 0.31144675 | -0.00037052 |

The geometric structure coordinates of TS* of T1*-T3* path under $E_x = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69943299 | 0.09531215 | -0.00008819 |
| C | 2.93679299 | -0.72902885 | -0.00045819 |
| C | 3.45270599 | 0.57612615 | -0.00047219 |
| C | 2.56350799 | 1.66688715 | -0.00029019 |
| C | 1.16846799 | 1.45800215 | -0.00009619 |
| C | -0.70227201 | -0.22068385 | 0.00010581 |
| C | -1.22050801 | -1.58565085 | 0.00013181 |
| C | -2.63150801 | -1.70737285 | 0.00032981 |
| C | -3.45253701 | -0.57001685 | 0.00048881 |
| C | -2.87257601 | 0.69643115 | 0.00045281 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.56787499 | -1.60448685 | -0.00059519 |
| H | 2.94636599 | 2.67845815 | -0.00030219 |
| H | -3.07589001 | -2.69426085 | 0.00035881 |
| H | -3.46664601 | 1.59889915 | 0.00057081 |
| O | -0.41421601 | -2.57205885 | -0.00001919 |
| H | 1.16452099 | -1.86193485 | -0.00024319 |
| O | 0.31271699 | 2.42948015 | 0.00007281 |
| H | -0.78505801 | 1.85836115 | 0.00020181 |
| N | 1.62313299 | -0.92247385 | -0.00027219 |
| N | -1.53011001 | 0.84563015 | 0.00026581 |
| C | -4.93260101 | -0.75810585 | 0.00069581 |
| C | 4.90300499 | 0.81892115 | -0.00067619 |
| O | 5.42734599 | 1.91464715 | -0.00069319 |
| O | -5.46132301 | -1.84372085 | 0.00074481 |
| C | -7.04787901 | 0.32968315 | 0.00101481 |
| C | -7.57844801 | 1.74624915 | 0.00111481 |
| H | -7.35910301 | -0.23310285 | 0.88372881 |
| H | -7.35934501 | -0.23306785 | -0.88163719 |
| H | -7.24336201 | 2.28732015 | -0.88641219 |
| H | -8.67074501 | 1.73030515 | 0.00126381 |
| H | -7.24311901 | 2.28728515 | 0.88857081 |
| C | 7.05171999 | -0.19512985 | -0.00106619 |
| C | 7.64746399 | -1.58930585 | -0.00123419 |
| H | 7.35206799 | 0.37922415 | 0.88029281 |
| H | 7.35179099 | 0.37931715 | -0.88245919 |
| H | 7.32895799 | -2.14406785 | -0.88672019 |
| H | 8.73974899 | -1.53221485 | -0.00140319 |
| H | 7.32923699 | -2.14416285 | 0.88429181 |
| O | 5.62122899 | -0.34520685 | -0.00085019 |
| O | -5.59213901 | 0.41251315 | 0.00081681 |

The geometric structure coordinates of TS* of N*-T2* path under $E_x = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.71096544 | 0.08424195 | 0.00000989 |
| C | 2.89413444 | -0.70956105 | -0.00018411 |
| C | 3.45005744 | 0.59723695 | 0.00008689 |
| C | 2.57268044 | 1.69236695 | 0.00032989 |
| C | 1.18846044 | 1.46337695 | 0.00029789 |
| C | -0.68283256 | -0.20410705 | -0.00003511 |
| C | -1.22577556 | -1.53626805 | -0.00031011 |
| C | -2.60954456 | -1.69534305 | -0.00032811 |
| C | -3.44129056 | -0.56803405 | -0.00008011 |
| C | -2.85349256 | 0.70963195 | 0.00018289 |
| H | 3.55219444 | -1.56951305 | -0.00037511 |
| H | 2.94893844 | 2.70643195 | 0.00054089 |
| H | -3.04138356 | -2.68771205 | -0.00053311 |
| H | -3.46516556 | 1.60193795 | 0.00037889 |
| O | -0.43279656 | -2.60231105 | -0.00054411 |
| H | 0.51373344 | -2.26805505 | -0.00048511 |
| O | 0.32666944 | 2.44128495 | 0.00051589 |
| H | -0.72453656 | 1.91704995 | 0.00041589 |
| N | 1.59473844 | -0.95790305 | -0.00022111 |
| N | -1.53767856 | 0.87229295 | 0.00020189 |
| C | -4.91289156 | -0.76753805 | -0.00010511 |
| C | 4.89630944 | 0.82800495 | 0.00011789 |
| O | 5.43239144 | 1.92124695 | 0.00034389 |
| O | -5.43437456 | -1.85883505 | -0.00033011 |
| C | -7.03636056 | 0.30506195 | 0.00014689 |
| C | -7.57898056 | 1.71702895 | 0.00045089 |
| H | -7.34330556 | -0.26076105 | 0.88258889 |
| H | -7.34332656 | -0.26038905 | -0.88252511 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.24849356 | 2.26113995 | -0.88695111 |
| H | -8.67109556 | 1.69175895 | 0.00045889 |
| H | -7.24847256 | 2.26076595 | 0.88807489 |
| C | 7.03968044 | -0.19610205 | -0.00012711 |
| C | 7.63106444 | -1.59252905 | -0.00043011 |
| H | 7.34396944 | 0.37704695 | 0.88103789 |
| H | 7.34394544 | 0.37741995 | -0.88105911 |
| H | 7.30978644 | -2.14599505 | -0.88575711 |
| H | 8.72374244 | -1.54002505 | -0.00043311 |
| H | 7.30980944 | -2.14637005 | 0.88467089 |
| O | 5.61084744 | -0.34143705 | -0.00013911 |
| O | -5.58184056 | 0.39953795 | 0.00014989 |

The geometric structure coordinates of TS* of T2*-T3* path under $E_x = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69161643 | 0.27832009 | 0.00000927 |
| C | 2.86021743 | -0.66145291 | 0.00110027 |
| C | 3.46905343 | 0.60596109 | 0.00046027 |
| C | 2.65155843 | 1.74944109 | -0.00042773 |
| C | 1.23607343 | 1.63599509 | -0.00067273 |
| C | -0.69213157 | -0.03939091 | -0.00022973 |
| C | -1.15625957 | -1.41300291 | 0.00045127 |
| C | -2.54794057 | -1.63158091 | 0.00030827 |
| C | -3.44381457 | -0.55623491 | -0.00051673 |
| C | -2.95395357 | 0.74905109 | -0.00119673 |
| H | 3.44611143 | -1.56985591 | 0.00182727 |
| H | 3.09238443 | 2.73726109 | -0.00088173 |
| H | -2.92449157 | -2.64606091 | 0.00079827 |
| H | -3.60107257 | 1.61346709 | -0.00188073 |
| O | -0.29936457 | -2.38204391 | 0.00115627 |
| H | 0.80990643 | -1.79892591 | 0.00116227 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.45117743 | 2.63406909 | -0.00146573 |
| H | -1.21722057 | 1.91283409 | -0.00148773 |
| N | 1.53592243 | -0.80112791 | 0.00087627 |
| N | -1.63362557 | 0.96624709 | -0.00105573 |
| C | -4.90804757 | -0.83907491 | -0.00069373 |
| C | 4.93079443 | 0.75057409 | 0.00074927 |
| O | 5.52886643 | 1.80827709 | 0.00022627 |
| O | -5.36437857 | -1.95672091 | -0.00016873 |
| C | -7.08794757 | 0.11614609 | -0.00170973 |
| C | -7.70475057 | 1.49708009 | -0.00268473 |
| H | -7.36291057 | -0.46435691 | 0.88148727 |
| H | -7.36251757 | -0.46542991 | -0.88432173 |
| H | -7.40433257 | 2.05735509 | -0.89068173 |
| H | -8.79388857 | 1.41309609 | -0.00286973 |
| H | -7.40471957 | 2.05843409 | 0.88476227 |
| C | 7.01000343 | -0.39919291 | 0.00203527 |
| C | 7.51582643 | -1.82869891 | 0.00315327 |
| H | 7.34728243 | 0.15527709 | 0.88297227 |
| H | 7.34775843 | 0.15406709 | -0.87948073 |
| H | 7.16236043 | -2.36266791 | -0.88183973 |
| H | 8.60963143 | -1.84202391 | 0.00345127 |
| H | 7.16189343 | -2.36144691 | 0.88869527 |
| O | 5.57412843 | -0.45802391 | 0.00168927 |
| O | -5.63866457 | 0.28820609 | -0.00148973 |

The geometric structure coordinates of N under $E_Y = +3 \times 10^{-3}$ a.u.

| | | | |
|---|------------|-------------|-------------|
| C | 0.72561200 | 0.16534300 | 0.00016500 |
| C | 2.88630500 | -0.70407800 | -0.00000400 |
| C | 3.45130000 | 0.57604600 | 0.00010100 |
| C | 2.60535000 | 1.67911700 | 0.00028000 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.22248000 | 1.49948400 | 0.00034500 |
| C | -0.71365300 | -0.13887200 | 0.00007400 |
| C | -1.20853100 | -1.47409100 | -0.00007700 |
| C | -2.59440200 | -1.65540500 | -0.00008100 |
| C | -3.43824700 | -0.55343000 | 0.00002000 |
| C | -2.87506300 | 0.72827400 | 0.00010600 |
| H | 3.50857700 | -1.58900000 | -0.00012700 |
| H | 3.01493600 | 2.68116100 | 0.00040800 |
| H | -3.00017700 | -2.65924300 | -0.00018900 |
| H | -3.50172400 | 1.61023000 | 0.00016600 |
| O | -0.42623100 | -2.55130300 | -0.00025900 |
| H | 0.51494300 | -2.22724400 | -0.00035600 |
| O | 0.42901000 | 2.57788700 | 0.00063000 |
| H | -0.50853300 | 2.23259500 | 0.00082500 |
| N | 1.57193000 | -0.88639900 | 0.00002500 |
| N | -1.56151400 | 0.91462600 | 0.00012800 |
| C | -4.91164200 | -0.78771600 | 0.00000400 |
| C | 4.92568300 | 0.80328100 | 0.00005900 |
| O | 5.44240400 | 1.89737900 | 0.00017300 |
| O | -5.42333600 | -1.87917900 | -0.00013600 |
| C | -7.05400300 | 0.22557300 | -0.00001300 |
| C | -7.63935500 | 1.62220500 | 0.00057300 |
| H | -7.34982900 | -0.34832800 | 0.88131100 |
| H | -7.34985600 | -0.34758300 | -0.88181800 |
| H | -7.32003300 | 2.17491400 | -0.88604100 |
| H | -8.73093200 | 1.56711700 | 0.00053600 |
| H | -7.32005600 | 2.17415300 | 0.88766900 |
| C | 7.05784800 | -0.25162600 | -0.00006500 |
| C | 7.60342000 | -1.66361200 | -0.00044300 |
| H | 7.36568700 | 0.31383000 | 0.88311100 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.36562700 | 0.31428900 | -0.88296600 |
| H | 7.27044200 | -2.20784000 | -0.88635700 |
| H | 8.69599700 | -1.64045700 | -0.00047300 |
| H | 7.27050300 | -2.20829500 | 0.88521500 |
| O | 5.61017400 | -0.35173100 | -0.00003600 |
| O | -5.61127700 | 0.36752800 | 0.00001100 |

The geometric structure coordinates of N* under $E_Y = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.70462700 | 0.16329900 | -0.00005400 |
| C | 2.87797000 | -0.69596300 | -0.00021400 |
| C | 3.45875700 | 0.59709100 | -0.00022400 |
| C | 2.60482800 | 1.70801600 | -0.00011700 |
| C | 1.22457900 | 1.51411900 | -0.00001800 |
| C | -0.69290800 | -0.12260000 | -0.00001700 |
| C | -1.21029700 | -1.48331700 | -0.00005600 |
| C | -2.59120600 | -1.68714400 | 0.00000100 |
| C | -3.44739700 | -0.57941700 | 0.00007300 |
| C | -2.87347300 | 0.71151800 | 0.00007900 |
| H | 3.51295000 | -1.57299000 | -0.00028900 |
| H | 3.00936900 | 2.71126800 | -0.00010100 |
| H | -2.98722300 | -2.69418500 | -0.00002300 |
| H | -3.51512600 | 1.58378900 | 0.00013300 |
| O | -0.39537700 | -2.52005700 | -0.00017700 |
| H | 0.55924100 | -2.15006900 | -0.00028200 |
| O | 0.41262400 | 2.56548000 | 0.00013200 |
| H | -0.53431000 | 2.19774000 | 0.00032100 |
| N | 1.57550400 | -0.90033700 | -0.00013800 |
| N | -1.56659000 | 0.93139900 | 0.00003800 |
| C | -4.90569200 | -0.79873700 | 0.00013300 |
| C | 4.91615000 | 0.80819300 | -0.00032800 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.44959900 | 1.90119800 | -0.00015300 |
| O | -5.43089600 | -1.88930300 | 0.00016300 |
| C | -7.04336300 | 0.23084900 | 0.00037700 |
| C | -7.62646400 | 1.62900200 | 0.00055800 |
| H | -7.34376100 | -0.34188100 | 0.88145500 |
| H | -7.34392700 | -0.34172100 | -0.88074900 |
| H | -7.30580200 | 2.18092700 | -0.88626800 |
| H | -8.71829100 | 1.57718100 | 0.00065400 |
| H | -7.30563900 | 2.18076500 | 0.88742600 |
| C | 7.04298700 | -0.26220000 | -0.00005700 |
| C | 7.58889400 | -1.67474700 | 0.00004200 |
| H | 7.35557300 | 0.30302200 | 0.88234800 |
| H | 7.35574400 | 0.30296600 | -0.88243600 |
| H | 7.25527800 | -2.21925100 | -0.88566700 |
| H | 8.68162700 | -1.65338400 | 0.00015000 |
| H | 7.25510300 | -2.21919500 | 0.88571900 |
| O | 5.59984100 | -0.36033000 | -0.00019500 |
| O | -5.60367100 | 0.36860700 | 0.00025300 |

The geometric structure coordinates of T1* under $E_Y = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.67081800 | 0.13660100 | -0.09588400 |
| C | 2.92878800 | -0.72936800 | -0.11484100 |
| C | 3.45756500 | 0.53540200 | 0.01801800 |
| C | 2.57652000 | 1.64616700 | 0.07167700 |
| C | 1.20507600 | 1.45834100 | 0.00678200 |
| C | -0.74203200 | -0.15052500 | -0.01643900 |
| C | -1.25955500 | -1.51811500 | 0.11930800 |
| C | -2.64095100 | -1.67584200 | 0.10404600 |
| C | -3.48984600 | -0.55426700 | 0.03247800 |
| C | -2.92694000 | 0.71034000 | -0.05438300 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.53733400 | -1.61824100 | -0.18315500 |
| H | 2.97656000 | 2.64690200 | 0.15139600 |
| H | -3.05883500 | -2.66682300 | 0.21398600 |
| H | -3.53702700 | 1.60301300 | -0.07025100 |
| O | -0.41219000 | -2.48536100 | 0.20836600 |
| H | 1.21300500 | -1.83643100 | -0.25394300 |
| O | 0.40028200 | 2.52608000 | 0.04718600 |
| H | -0.53416300 | 2.19042800 | -0.03862900 |
| N | 1.59582800 | -0.89325400 | -0.19991700 |
| N | -1.60458000 | 0.87216100 | -0.11113900 |
| C | -4.95370700 | -0.77529900 | 0.07383600 |
| C | 4.91796500 | 0.76492200 | 0.07397600 |
| O | 5.42647200 | 1.85952400 | 0.18350100 |
| O | -5.47638100 | -1.85992700 | 0.17461000 |
| C | -7.09332300 | 0.24310700 | 0.01718400 |
| C | -7.67918500 | 1.63696500 | -0.07556400 |
| H | -7.37974300 | -0.26446200 | 0.94157200 |
| H | -7.40483700 | -0.39153200 | -0.81614300 |
| H | -7.37067900 | 2.12410700 | -1.00357500 |
| H | -8.77084200 | 1.58399600 | -0.05780200 |
| H | -7.34795000 | 2.25117200 | 0.76522700 |
| C | 7.06268100 | -0.26771600 | 0.05269000 |
| C | 7.63147100 | -1.66522800 | -0.07231300 |
| H | 7.33488000 | 0.20775500 | 0.99857200 |
| H | 7.39216700 | 0.38868000 | -0.75684700 |
| H | 7.33789600 | -2.12018600 | -1.02053400 |
| H | 8.72291800 | -1.62858600 | -0.03145700 |
| H | 7.27845600 | -2.30225100 | 0.74111300 |
| O | 5.61942200 | -0.38526200 | -0.00610900 |
| O | -5.65368000 | 0.38316500 | -0.01410400 |

The geometric structure coordinates of T2* under $E_Y = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.75076800 | 0.14973800 | 0.00046500 |
| C | 2.93268400 | -0.68384500 | 0.02979000 |
| C | 3.49233700 | 0.58991600 | -0.02724700 |
| C | 2.63247700 | 1.69881800 | -0.09821600 |
| C | 1.23470600 | 1.53240100 | -0.13504800 |
| C | -0.67126500 | -0.16133800 | 0.08802100 |
| C | -1.19905000 | -1.47356600 | -0.03649800 |
| C | -2.58374800 | -1.65616900 | -0.10210700 |
| C | -3.44495400 | -0.54188900 | -0.03205900 |
| C | -2.90446700 | 0.72627800 | 0.10828500 |
| H | 3.54936300 | -1.57202800 | 0.01389800 |
| H | 3.04052000 | 2.69449700 | -0.21124000 |
| H | -2.98931100 | -2.65532300 | -0.18030100 |
| H | -3.51342900 | 1.61453000 | 0.18240800 |
| O | -0.41101500 | -2.54238200 | -0.08649600 |
| H | 0.52789700 | -2.22899500 | 0.01470100 |
| O | 0.40879600 | 2.50548400 | -0.23936700 |
| H | -1.12772800 | 1.81430400 | 0.15340000 |
| N | 1.60177700 | -0.87229300 | 0.09140800 |
| N | -1.57756600 | 0.88179300 | 0.19936700 |
| C | -4.91018600 | -0.76026000 | -0.07534700 |
| C | 4.95793000 | 0.80833600 | -0.05861800 |
| O | 5.48171300 | 1.89839400 | -0.14574600 |
| O | -5.42798400 | -1.84453400 | -0.19298400 |
| C | -7.04926900 | 0.26487800 | -0.01921600 |
| C | -7.63112000 | 1.65873700 | 0.09297400 |
| H | -7.36659900 | -0.38291500 | 0.80151800 |
| H | -7.32968000 | -0.22632000 | -0.95409100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.29262900 | 2.28625200 | -0.73501500 |
| H | -8.72262100 | 1.60905800 | 0.06622000 |
| H | -7.32915900 | 2.12909000 | 1.03176200 |
| C | 7.09009200 | -0.24758500 | -0.00327700 |
| C | 7.63955300 | -1.65402400 | 0.10985000 |
| H | 7.41036100 | 0.39094800 | 0.82424600 |
| H | 7.38853200 | 0.24090400 | -0.93468600 |
| H | 7.29726000 | -2.27230700 | -0.72240800 |
| H | 8.73210600 | -1.63053800 | 0.09484800 |
| H | 7.31764400 | -2.12177800 | 1.04246000 |
| O | 5.64560400 | -0.34921900 | 0.02331900 |
| O | -5.60778200 | 0.39914600 | 0.02351000 |

The geometric structure coordinates of T3* in under $E_Y = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.69230800 | 0.17649900 | -0.00019700 |
| C | 2.92779000 | -0.69564600 | -0.00007300 |
| C | 3.47387400 | 0.59165400 | -0.00001300 |
| C | 2.61745800 | 1.69898000 | -0.00005300 |
| C | 1.20306900 | 1.55094500 | -0.00022200 |
| C | -0.68150000 | -0.15511100 | -0.00005100 |
| C | -1.19522500 | -1.53013400 | 0.00000000 |
| C | -2.60949800 | -1.68313100 | 0.00014500 |
| C | -3.46320800 | -0.57288500 | 0.00019200 |
| C | -2.91938600 | 0.71143500 | 0.00014600 |
| H | 3.53562200 | -1.58808000 | -0.00008900 |
| H | 3.02894800 | 2.69953600 | -0.00003100 |
| H | -3.01852500 | -2.68490100 | 0.00022800 |
| H | -3.52928900 | 1.60214300 | 0.00015400 |
| O | -0.39559300 | -2.51022400 | -0.00007000 |
| H | 1.13655900 | -1.79705600 | -0.00015800 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.40634100 | 2.53898100 | -0.00030100 |
| H | -1.12091100 | 1.81543300 | -0.00002400 |
| N | 1.60319700 | -0.86047100 | -0.00018000 |
| N | -1.59000200 | 0.88110200 | 0.00001700 |
| C | -4.93052100 | -0.78532500 | 0.00028300 |
| C | 4.94086200 | 0.79954900 | 0.00007100 |
| O | 5.47333200 | 1.88826400 | 0.00014600 |
| O | -5.45908200 | -1.87031300 | 0.00022800 |
| C | -7.06232600 | 0.25738000 | 0.00046700 |
| C | -7.63514800 | 1.65955300 | 0.00037800 |
| H | -7.36546700 | -0.31292900 | 0.88187700 |
| H | -7.36548600 | -0.31302400 | -0.88086800 |
| H | -7.31078900 | 2.20922400 | -0.88649600 |
| H | -8.72724200 | 1.61501500 | -0.00010100 |
| H | -7.31153800 | 2.20908900 | 0.88760100 |
| C | 7.06411600 | -0.27987000 | 0.00011000 |
| C | 7.60128400 | -1.69541900 | -0.00033500 |
| H | 7.37780100 | 0.28310900 | 0.88311600 |
| H | 7.37789900 | 0.28373100 | -0.88246000 |
| H | 7.26496000 | -2.23787300 | -0.88625000 |
| H | 8.69402600 | -1.67964500 | -0.00090700 |
| H | 7.26588100 | -2.23820700 | 0.88572400 |
| O | 5.61784500 | -0.36962300 | 0.00005500 |
| O | -5.62005100 | 0.38499300 | 0.00042900 |

The geometric structure coordinates of N under $E_z = +3 \times 10^{-3}$ a.u.

| | | | |
|---|------------|-------------|------------|
| C | 0.72021500 | 0.14973900 | 0.21426300 |
| C | 2.87786400 | -0.72416300 | 0.15246300 |
| C | 3.44589900 | 0.55463000 | 0.17707600 |
| C | 2.60497400 | 1.65888200 | 0.22956500 |

| | | | |
|---|-------------|-------------|-------------|
| C | 1.22019000 | 1.48243000 | 0.23873300 |
| C | -0.72021500 | -0.14975800 | 0.21423700 |
| C | -1.22016500 | -1.48246400 | 0.23831900 |
| C | -2.60494600 | -1.65894000 | 0.22915200 |
| C | -3.44589300 | -0.55468700 | 0.17702500 |
| C | -2.87788100 | 0.72412300 | 0.15277200 |
| H | 3.49934500 | -1.60865900 | 0.10875000 |
| H | 3.01572400 | 2.66035700 | 0.24720200 |
| H | -3.01567600 | -2.66042800 | 0.24649900 |
| H | -3.49938100 | 1.60862100 | 0.10934300 |
| O | -0.43506900 | -2.56203400 | 0.27306300 |
| H | 0.50449200 | -2.23120000 | 0.22669700 |
| O | 0.43512000 | 2.56200800 | 0.27384600 |
| H | -0.50445100 | 2.23120600 | 0.22743900 |
| N | 1.56366400 | -0.90512800 | 0.18064200 |
| N | -1.56368300 | 0.90510400 | 0.18095800 |
| C | -4.92037500 | -0.78101400 | 0.14612500 |
| C | 4.92038500 | 0.78093900 | 0.14619000 |
| O | 5.44200400 | 1.86142800 | 0.28629100 |
| O | -5.44197000 | -1.86155100 | 0.28593200 |
| C | -7.04315200 | 0.23808300 | -0.16449900 |
| C | -7.58914900 | 1.61867000 | -0.46049200 |
| H | -7.42598100 | -0.17007000 | 0.77463200 |
| H | -7.27458900 | -0.47739200 | -0.95672000 |
| H | -7.17934100 | 2.00282200 | -1.39652500 |
| H | -8.67716900 | 1.57584400 | -0.55367600 |
| H | -7.33643300 | 2.31674800 | 0.34095500 |
| C | 7.04313000 | -0.23810300 | -0.16483000 |
| C | 7.58908800 | -1.61861000 | -0.46126900 |
| H | 7.42600800 | 0.16975400 | 0.77441000 |

| | | | |
|---|-------------|-------------|-------------|
| H | 7.27454700 | 0.47761100 | -0.95684200 |
| H | 7.17923200 | -2.00246800 | -1.39740300 |
| H | 8.67710500 | -1.57577700 | -0.55448700 |
| H | 7.33639200 | -2.31692900 | 0.33997300 |
| O | 5.60094400 | -0.36109100 | -0.06181000 |
| O | -5.60096300 | 0.36106900 | -0.06150400 |

The geometric structure coordinates of N* under $E_z = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|------------|
| C | 0.69856800 | 0.14141400 | 0.11994000 |
| C | 2.87408600 | -0.70834800 | 0.08732700 |
| C | 3.45356000 | 0.58266100 | 0.11567000 |
| C | 2.60049400 | 1.69287300 | 0.14732900 |
| C | 1.21967200 | 1.49635700 | 0.14017100 |
| C | -0.69856900 | -0.14154500 | 0.11990800 |
| C | -1.21970100 | -1.49649000 | 0.13968600 |
| C | -2.60052800 | -1.69297800 | 0.14682600 |
| C | -3.45357100 | -0.58273700 | 0.11557500 |
| C | -2.87407100 | 0.70826800 | 0.08765100 |
| H | 3.51120600 | -1.58326800 | 0.05372000 |
| H | 3.00228400 | 2.69723500 | 0.16152800 |
| H | -3.00233800 | -2.69733700 | 0.16069200 |
| H | -3.51117400 | 1.58321200 | 0.05436500 |
| O | -0.40800000 | -2.54153100 | 0.16010500 |
| H | 0.54290200 | -2.17513800 | 0.12514800 |
| O | 0.40794300 | 2.54137300 | 0.16099400 |
| H | -0.54294900 | 2.17497400 | 0.12598300 |
| N | 1.56951700 | -0.91896200 | 0.10010600 |
| N | -1.56949600 | 0.91885300 | 0.10046200 |
| C | -4.91182100 | -0.79555100 | 0.11028300 |
| C | 4.91180500 | 0.79550600 | 0.11040100 |

| | | | |
|---|-------------|-------------|-------------|
| O | 5.44336500 | 1.88229500 | 0.20496800 |
| O | -5.44340000 | -1.88235900 | 0.20450300 |
| C | -7.03880600 | 0.24643700 | -0.09198100 |
| C | -7.59544500 | 1.64055200 | -0.29255100 |
| H | -7.40285500 | -0.21776000 | 0.82903100 |
| H | -7.29142500 | -0.42125700 | -0.91934600 |
| H | -7.20942700 | 2.08082400 | -1.21406700 |
| H | -8.68552400 | 1.60076200 | -0.36121200 |
| H | -7.32359200 | 2.29102600 | 0.54227300 |
| C | 7.03880400 | -0.24637200 | -0.09229700 |
| C | 7.59546000 | -1.64040900 | -0.29336400 |
| H | 7.40287900 | 0.21751700 | 0.82886000 |
| H | 7.29138100 | 0.42160900 | -0.91944300 |
| H | 7.20941700 | -2.08037300 | -1.21501500 |
| H | 8.68553600 | -1.60057600 | -0.36205100 |
| H | 7.32365000 | -2.29117200 | 0.54124800 |
| O | 5.59903000 | -0.36701800 | -0.01561600 |
| O | -5.59902700 | 0.36703200 | -0.01531200 |

The geometric structure coordinates of T1* under $E_z = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.67535600 | 0.20050000 | 0.09618700 |
| C | 2.89544700 | -0.71556500 | -0.05209900 |
| C | 3.45206400 | 0.52664900 | 0.18232400 |
| C | 2.61088000 | 1.64735900 | 0.36004000 |
| C | 1.22426300 | 1.48626000 | 0.29754600 |
| C | -0.75233700 | -0.08632500 | 0.19997300 |
| C | -1.23154400 | -1.45281000 | 0.43630400 |
| C | -2.62271600 | -1.62984700 | 0.39064000 |
| C | -3.48292500 | -0.53148100 | 0.22010000 |
| C | -2.93295200 | 0.73585000 | 0.07876000 |

| | | | |
|---|-------------|-------------|-------------|
| H | 3.48929100 | -1.60074500 | -0.22123200 |
| H | 3.03518400 | 2.63173600 | 0.49529900 |
| H | -3.03100500 | -2.61464700 | 0.57417700 |
| H | -3.55430100 | 1.61818800 | 0.01176800 |
| O | -0.39011100 | -2.40055700 | 0.63364800 |
| H | 1.12928300 | -1.78027300 | -0.12975700 |
| O | 0.44412800 | 2.56324800 | 0.43058000 |
| H | -0.48597100 | 2.28059300 | 0.24028500 |
| N | 1.55842300 | -0.84870000 | -0.12340400 |
| N | -1.60248000 | 0.92225900 | 0.02842100 |
| C | -4.94905200 | -0.76350300 | 0.23453400 |
| C | 4.92358400 | 0.71916600 | 0.21188400 |
| O | 5.45961500 | 1.76867600 | 0.48354200 |
| O | -5.46601700 | -1.82675800 | 0.49289500 |
| C | -7.08389100 | 0.20791900 | -0.14558000 |
| C | -7.64534300 | 1.54262400 | -0.58850300 |
| H | -7.45193800 | -0.09248800 | 0.83938000 |
| H | -7.32355000 | -0.59413300 | -0.84754000 |
| H | -7.25164900 | 1.81998000 | -1.56821800 |
| H | -8.73435100 | 1.48372300 | -0.65976500 |
| H | -7.38619400 | 2.32929500 | 0.12394200 |
| C | 7.04079500 | -0.30739200 | -0.12658500 |
| C | 7.57828100 | -1.66274000 | -0.53456700 |
| H | 7.39204000 | -0.00052300 | 0.86225500 |
| H | 7.31656000 | 0.47705600 | -0.83512200 |
| H | 7.20340900 | -1.94622200 | -1.51993500 |
| H | 8.66980200 | -1.63217500 | -0.57871100 |
| H | 7.28186100 | -2.43076100 | 0.18370700 |
| O | 5.59520700 | -0.41213000 | -0.09308400 |
| O | -5.64360600 | 0.35045600 | -0.07988800 |

The geometric structure coordinates of T2* under $E_z = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|-------------|
| C | 0.75265400 | 0.09325400 | 0.18976500 |
| C | 2.93325000 | -0.73476900 | 0.07135000 |
| C | 3.48520900 | 0.53025700 | 0.22179600 |
| C | 2.62666700 | 1.63007300 | 0.39412100 |
| C | 1.23645000 | 1.45702900 | 0.43288800 |
| C | -0.67332400 | -0.19181500 | 0.08163200 |
| C | -1.22188400 | -1.47869400 | 0.28878200 |
| C | -2.60671200 | -1.64135500 | 0.35674000 |
| C | -3.45182800 | -0.52305700 | 0.17654600 |
| C | -2.89879900 | 0.71735500 | -0.06885100 |
| H | 3.55225000 | -1.61852400 | 0.00130700 |
| H | 3.03708100 | 2.61272400 | 0.58372500 |
| H | -3.02859000 | -2.62565400 | 0.49992800 |
| H | -3.49416400 | 1.60023800 | -0.24410000 |
| O | -0.43985700 | -2.55386100 | 0.42525800 |
| H | 0.48950900 | -2.27088700 | 0.23187400 |
| O | 0.39513100 | 2.40622200 | 0.62870700 |
| H | -1.14466500 | 1.78459400 | -0.18683400 |
| N | 1.60392800 | -0.91528000 | 0.01614400 |
| N | -1.56122200 | 0.85256900 | -0.14310700 |
| C | -4.92255400 | -0.71818900 | 0.21470300 |
| C | 4.95134800 | 0.75953900 | 0.24322500 |
| O | 5.46959500 | 1.82035600 | 0.50944300 |
| O | -5.45524500 | -1.76779300 | 0.49240600 |
| C | -7.04355500 | 0.30309100 | -0.11584500 |
| C | -7.58611600 | 1.65735200 | -0.52075400 |
| H | -7.38882700 | -0.00456600 | 0.87483400 |
| H | -7.32159800 | -0.48185200 | -0.82296100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -7.21729400 | 1.94176500 | -1.50814000 |
| H | -8.67780000 | 1.62454400 | -0.55887700 |
| H | -7.28731700 | 2.42587400 | 0.19599900 |
| C | 7.08585900 | -0.21379100 | -0.13370200 |
| C | 7.64635300 | -1.54604600 | -0.58518900 |
| H | 7.45083400 | 0.07793300 | 0.85502600 |
| H | 7.32986400 | 0.59336300 | -0.82827600 |
| H | 7.25591300 | -1.81462800 | -1.56864400 |
| H | 8.73576000 | -1.48887600 | -0.65171300 |
| H | 7.38275100 | -2.33793000 | 0.11979900 |
| O | 5.64517300 | -0.35401100 | -0.07458800 |
| O | -5.59809400 | 0.41088200 | -0.09021600 |

The geometric structure coordinates of T3* in under $E_Z = +3 \times 10^{-3}$ a.u.

| | | | |
|---|-------------|-------------|------------|
| C | 0.68786800 | 0.16468200 | 0.18998500 |
| C | 2.92682100 | -0.70735100 | 0.11364100 |
| C | 3.47610800 | 0.57494400 | 0.15598000 |
| C | 2.62404100 | 1.68280800 | 0.22354000 |
| C | 1.20834400 | 1.53757800 | 0.23554000 |
| C | -0.68782900 | -0.16467300 | 0.18994800 |
| C | -1.20829400 | -1.53759900 | 0.23505800 |
| C | -2.62398900 | -1.68283700 | 0.22306500 |
| C | -3.47607200 | -0.57495700 | 0.15595400 |
| C | -2.92679800 | 0.70735900 | 0.11411300 |
| H | 3.53132100 | -1.59987800 | 0.05392200 |
| H | 3.03573100 | 2.68284200 | 0.25453000 |
| H | -3.03566800 | -2.68288700 | 0.25366500 |
| H | -3.53131200 | 1.59990600 | 0.05484100 |
| O | -0.42047500 | -2.52647400 | 0.29237000 |
| H | 1.14631300 | -1.80743200 | 0.14729700 |

| | | | |
|---|-------------|-------------|-------------|
| O | 0.42053000 | 2.52644300 | 0.29319600 |
| H | -1.14624600 | 1.80744900 | 0.14800600 |
| N | 1.59913200 | -0.87118200 | 0.14129700 |
| N | -1.59910300 | 0.87120700 | 0.14177100 |
| C | -4.94389900 | -0.78152300 | 0.12820700 |
| C | 4.94392500 | 0.78149300 | 0.12823900 |
| O | 5.47980000 | 1.85944500 | 0.24535600 |
| O | -5.47975500 | -1.85951600 | 0.24499700 |
| C | -7.05994400 | 0.26846500 | -0.14580500 |
| C | -7.59934600 | 1.65960800 | -0.40367300 |
| H | -7.44272200 | -0.16067100 | 0.78420200 |
| H | -7.30203200 | -0.42477700 | -0.95469000 |
| H | -7.19336900 | 2.06486800 | -1.33261700 |
| H | -8.68822100 | 1.62638100 | -0.49105300 |
| H | -7.33766600 | 2.33593100 | 0.41363000 |
| C | 7.05990400 | -0.26851000 | -0.14620500 |
| C | 7.59922500 | -1.65962900 | -0.40436600 |
| H | 7.44274700 | 0.16043800 | 0.78386000 |
| H | 7.30197000 | 0.42487400 | -0.95497600 |
| H | 7.19314400 | -2.06471300 | -1.33334200 |
| H | 8.68809100 | -1.62642300 | -0.49184800 |
| H | 7.33760100 | -2.33608600 | 0.41284300 |
| O | 5.61832600 | -0.37897000 | -0.04745900 |
| O | -5.61836500 | 0.37896100 | -0.04711700 |