

Computational Supporting Information

Photochemical synthesis of 1,2,4-triazoles via addition reaction of triplet intermediates to diazoalkanes and azomethine ylide intermediates

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Table of Contents

| | |
|---|-----|
| 1. Computational Detail | S1 |
| 2. Computed Reaction Pathways | S2 |
| 3. Computed Energy of all Stationary Points | S4 |
| 4. 3D Structures and Coordinates of all Stationary Points | S5 |
| 5. References | S14 |

1. Computational Details

All calculations were performed using the Gaussian 16, Revision B.01 package.¹ The (U)M06-2X functional² together with Grimme's dispersion correction³ (denoted (U)M06-2X-D3) and the def2-SVP basis set⁴ were applied for the optimization of all stationary points in acetonitrile, in which the solvent effects ($\epsilon = 35.688$) were evaluated by SMD solvation model.⁵ Analytical frequency calculations were carried out at the same level of theory in order to confirm each stationary point as either an intermediate (no imaginary frequencies) or a transition state (only one imaginary frequency). Key transition-state structures were confirmed to connect corresponding reactants and products by intrinsic reaction coordinate (IRC) calculations.⁶ To improve the calculation accuracy, single point energy calculations using larger def2-TZVPP basis set⁴ at the (U)M06-2X-D3 level with SMD solvation model were performed based on the optimized geometries of all species. Standard state concentrations of 1.0 mol/L were used for all species in calculations. The given Gibbs free energies in Table S2 were calculated according to the formula: $G_{\text{sol}} = \text{TCG} + E_{\text{sol}}$ (kcal/mol). The CYL View software was employed to show the 3D structures of the studied species.⁷ Vertical excitations energies were calculated at the TD-M06-2X-D3 level with the def2-TZVPP basis set. The searching for minimal energy crossing points (MECPs) was conducted using a modified version of Harvey's code⁸ (sobMECP software)⁹ interfaced with Gaussian 16.

2. Computed Reaction Pathways

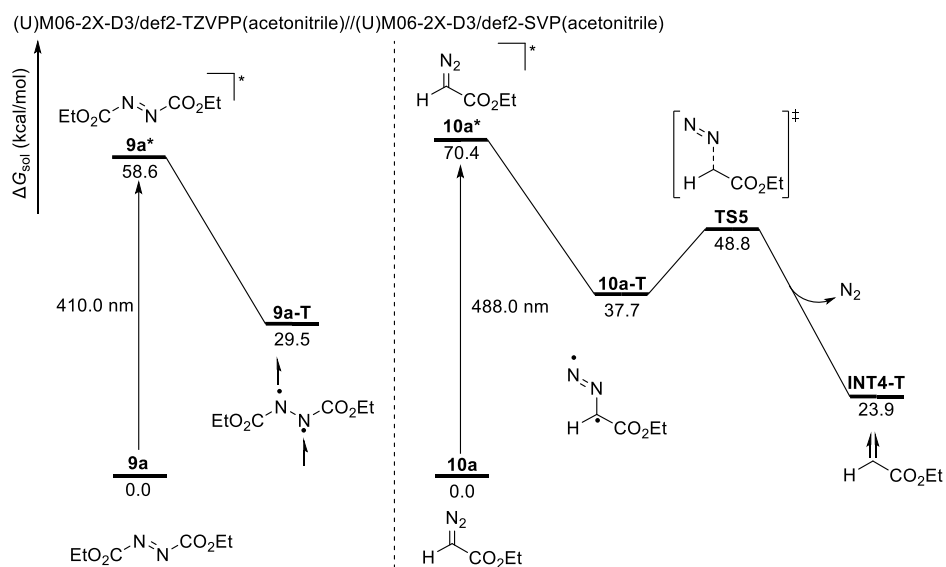


Figure S1. Computational photochemical properties of EDA and DEAD.

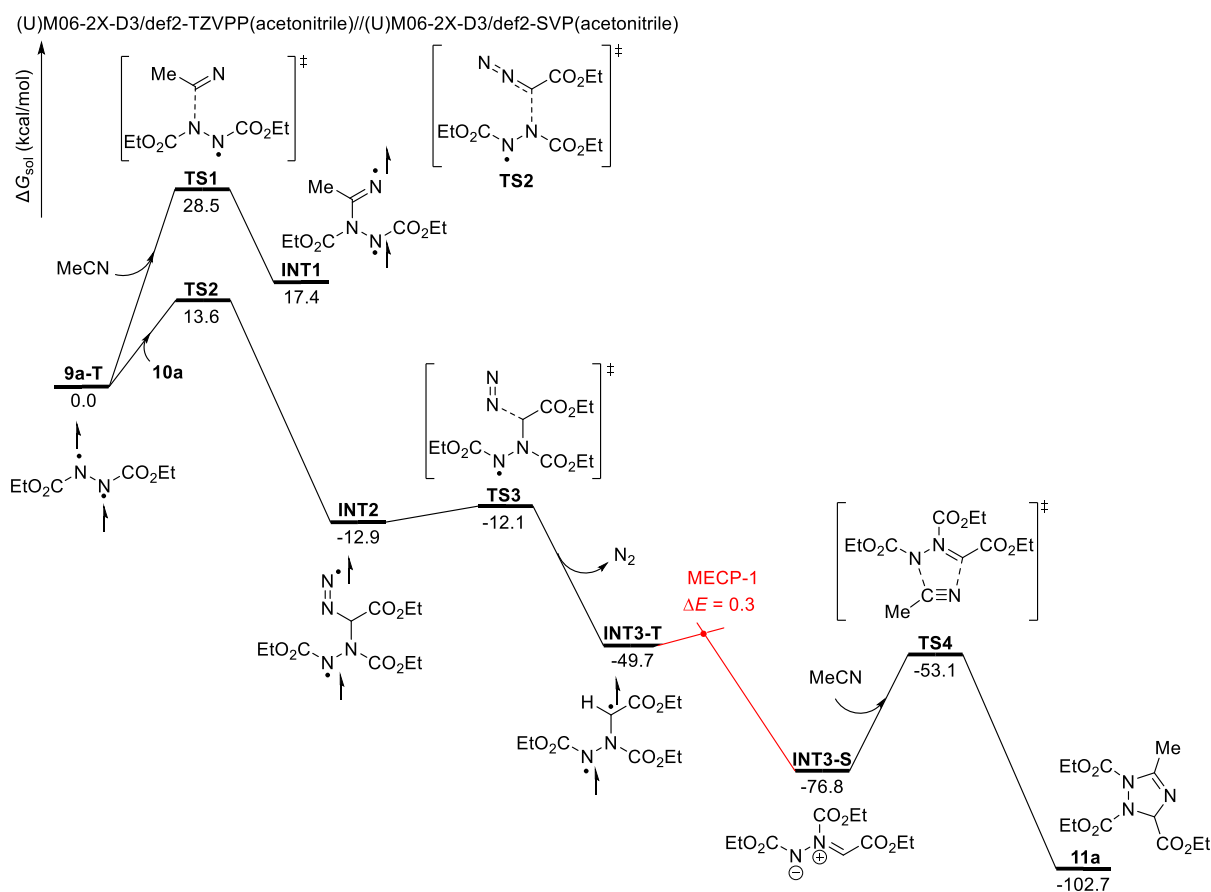


Figure S2. Relative free-energy profile for the reaction from triplet state of DEAD.

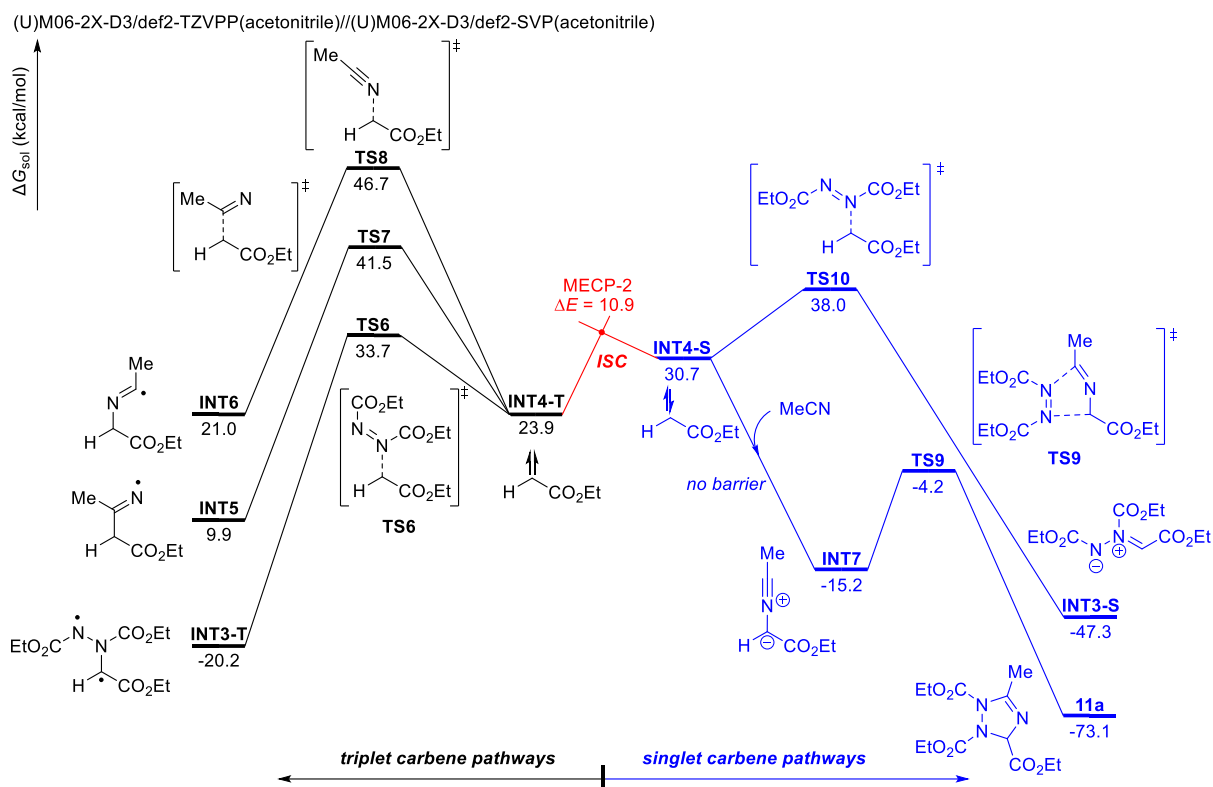


Figure S3. Relative free-energy profile for the reaction from free carbene.

Table S1. Single point energies (E) of MECP

| Name | E (a.u.) | ΔE (kcal/mol) |
|--------|-------------|-----------------------|
| INT3-T | -950.383085 | - |
| MECP-1 | -950.382585 | 0.3 |
| INT4-T | -305.998752 | - |
| MECP-2 | -305.981362 | 10.9 |

3. Computed Energy of all Stationary Points

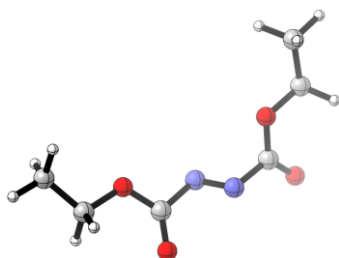
Table S2. Calculated energies of all stationary points.

Thermal correction to Gibbs free energies (*TCG*, in Hartree), thermal correction to enthalpies (*TCH*, in Hartree), sum of electronic and thermal free energies (*G*, in Hartree), single point energies in acetonitrile computed at the (U)M06-2X-D3/def2-TZVPP level (*E*, in Hartree), and the total spin-squared operator of open-shell species *S*².

| Name | <i>TCG</i> /a.u. | <i>TCH</i> /a.u. | <i>G</i> /a.u. | <i>E</i> /a.u. | <i>S</i> ² |
|----------------------|------------------|------------------|----------------|----------------|-----------------------|
| 9a | 0.129908 | 0.187141 | -644.145194 | -645.033374 | - |
| 9a-T | 0.127903 | 0.186466 | -644.103860 | -644.984285 | 2.0099 |
| MeCN | 0.022521 | 0.050010 | -132.577474 | -132.758347 | - |
| TS1 | 0.170183 | 0.236502 | -776.641453 | -777.716925 | 2.0305 |
| INT1 | 0.173640 | 0.239004 | -776.661115 | -777.738132 | 2.0200 |
| 10a | 0.072134 | 0.115368 | -415.389919 | -415.950171 | - |
| TS2 | 0.224629 | 0.302828 | -1059.477540 | -1060.937424 | 2.0250 |
| INT2 | 0.227981 | 0.305559 | -1059.522360 | -1060.983032 | 2.0112 |
| TS3 | 0.223129 | 0.302848 | -1059.518698 | -1060.976784 | 2.0178 |
| N₂ | -0.012541 | 0.009192 | -109.409372 | -109.530558 | - |
| INT3-T | 0.218294 | 0.292687 | -950.164791 | -951.488859 | 2.0129 |
| INT3-S | 0.222059 | 0.294539 | -950.205915 | -951.535835 | - |
| TS4 | 0.266896 | 0.345978 | -1082.749822 | -1084.275836 | - |
| 11a | 0.272057 | 0.349832 | -1082.838061 | -1084.362809 | - |
| 10a-T | 0.068716 | 0.113258 | -415.330948 | -415.886663 | 2.0322 |
| TS5 | 0.063461 | 0.110383 | -415.309322 | -415.863686 | 2.0268 |
| INT4-T | 0.061858 | 0.101093 | -305.936894 | -306.358756 | 2.0118 |
| INT4-S | 0.061492 | 0.100870 | -305.921696 | -306.347578 | - |
| TS6 | 0.215144 | 0.289151 | -950.073755 | -951.399764 | 2.0545 |
| TS7 | 0.100828 | 0.151695 | -438.489337 | -439.105513 | 2.0310 |
| INT5 | 0.106319 | 0.154691 | -438.543666 | -439.161288 | 2.0503 |
| TS8 | 0.097916 | 0.151465 | -438.480740 | -439.094251 | 2.0303 |
| INT6 | 0.104061 | 0.154628 | -438.526100 | -439.141405 | 2.0301 |
| INT7 | 0.107005 | 0.156076 | -438.583535 | -439.201929 | - |
| TS9 | 0.265098 | 0.344297 | -1082.721511 | -1084.245982 | - |
| TS10 | 0.213249 | 0.289153 | -950.064130 | -951.391077 | - |

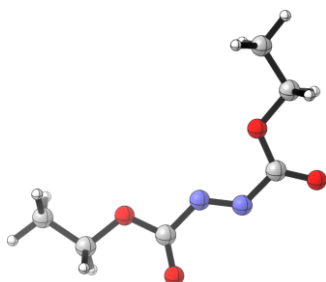
4. 3D Structures and Coordinates of all Stationary Points

9a



| | | | |
|---|-------------|-------------|-------------|
| N | -0.31088700 | -0.47190100 | -0.37837100 |
| N | 0.48170100 | -1.01368100 | 0.38633900 |
| C | 1.85388100 | -0.86577800 | -0.03368400 |
| C | -1.69398400 | -0.69767100 | 0.02132500 |
| O | -2.11047800 | -1.73701100 | 0.43629100 |
| O | 2.47196100 | -1.80317300 | -0.44264200 |
| O | 2.27642700 | 0.35670500 | 0.16682400 |
| C | 3.66808600 | 0.61393200 | -0.12944900 |
| H | 3.82892200 | 0.42446300 | -1.19996400 |
| H | 4.27690100 | -0.09954600 | 0.44346600 |
| C | 3.95943600 | 2.04321700 | 0.24548700 |
| H | 5.01235300 | 2.26657500 | 0.02725600 |
| H | 3.32965600 | 2.73402500 | -0.33177500 |
| H | 3.78239300 | 2.20915300 | 1.31702900 |
| C | -3.77305000 | 0.37339500 | 0.11570900 |
| H | -3.87624600 | 0.10950500 | 1.17787600 |
| H | -4.24319900 | -0.42010600 | -0.48268700 |
| O | -2.36694500 | 0.40293700 | -0.20769100 |
| C | -4.34485600 | 1.73269400 | -0.19119300 |
| H | -4.22231700 | 1.97613700 | -1.25552200 |
| H | -5.41717100 | 1.73645600 | 0.04592300 |
| H | -3.85177500 | 2.50800900 | 0.41120300 |

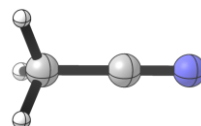
9a-T



| | | | |
|---|-------------|-------------|-------------|
| N | -0.32230400 | -0.41695900 | -0.10387300 |
| N | 0.61566400 | -1.22245800 | -0.08381100 |
| C | 1.98794700 | -0.94571800 | -0.03211600 |
| C | -1.69283200 | -0.70330900 | 0.01153100 |
| O | -2.13519500 | -1.81061700 | 0.13862000 |
| O | 2.80744700 | -1.82181300 | -0.02017500 |
| O | 2.22147400 | 0.35615300 | -0.00399200 |
| C | 3.60854600 | 0.74412400 | 0.03903900 |

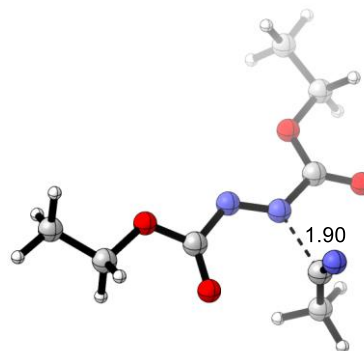
| | | | |
|---|-------------|-------------|-------------|
| H | 4.11539900 | 0.31876300 | -0.83892500 |
| H | 4.06316700 | 0.30898100 | 0.94055200 |
| C | 3.66009800 | 2.25012800 | 0.04853300 |
| H | 4.70794600 | 2.57752100 | 0.08145800 |
| H | 3.19428700 | 2.66147800 | -0.85758800 |
| H | 3.14106100 | 2.65237300 | 0.92944800 |
| C | -3.80043000 | 0.31091900 | 0.05117200 |
| H | -4.04355700 | -0.17645500 | 1.00630200 |
| H | -4.15493700 | -0.33659900 | -0.76370800 |
| O | -2.36814200 | 0.42531100 | -0.04930500 |
| C | -4.37790600 | 1.69964200 | -0.03865500 |
| H | -4.11685600 | 2.16899700 | -0.99717900 |
| H | -5.47218300 | 1.64324300 | 0.03529700 |
| H | -4.00505900 | 2.33062600 | 0.77991800 |

MeCN



| | | | |
|---|-------------|-------------|-------------|
| C | 0.00000000 | 0.00000000 | -1.17783800 |
| H | 0.00000000 | 1.03373300 | -1.54589400 |
| H | -0.89523900 | -0.51686600 | -1.54589400 |
| H | 0.89523900 | -0.51686600 | -1.54589400 |
| C | 0.00000000 | 0.00000000 | 0.27924200 |
| N | 0.00000000 | 0.00000000 | 1.43275100 |

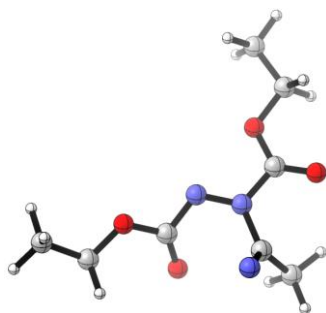
TS1



| | | | |
|---|-------------|-------------|-------------|
| N | 0.36729000 | 0.32757800 | 0.02792000 |
| N | -0.55576500 | -0.53018100 | -0.08694000 |
| C | -1.93183200 | -0.21873400 | -0.07561500 |
| C | 1.70308800 | -0.07030800 | 0.07828000 |
| O | 2.09066200 | -1.20331000 | 0.22950400 |
| O | -2.76758300 | -1.07927300 | -0.13377300 |
| O | -2.13813500 | 1.07814100 | 0.00618000 |
| C | -3.51873100 | 1.49556500 | 0.03206900 |
| H | -4.00397900 | 1.03072400 | 0.90204800 |
| H | -4.01065000 | 1.12050600 | -0.87644100 |

| | | | |
|---|-------------|-------------|-------------|
| C | -3.53700900 | 3.00009400 | 0.10739900 |
| H | -4.57804200 | 3.34930800 | 0.12944900 |
| H | -3.03166300 | 3.35120300 | 1.01757700 |
| H | -3.03991100 | 3.43983800 | -0.76820400 |
| C | 3.89119500 | 0.76242300 | 0.04491000 |
| H | 4.17325500 | 0.06413200 | -0.75654700 |
| H | 4.11681800 | 0.28086800 | 1.00765200 |
| O | 2.47595800 | 0.99694500 | -0.02848100 |
| C | 4.58561100 | 2.09275500 | -0.09678300 |
| H | 4.28773500 | 2.77571700 | 0.71083000 |
| H | 5.67263900 | 1.94470500 | -0.04498300 |
| H | 4.34286200 | 2.55789300 | -1.06226300 |
| C | -0.38732800 | -2.90301100 | 1.10278600 |
| H | -1.37169400 | -2.65965500 | 1.52255800 |
| H | 0.39899800 | -2.41941900 | 1.69389700 |
| H | -0.24130100 | -3.98984400 | 1.09399000 |
| C | -0.32099200 | -2.40584700 | -0.28878700 |
| N | -0.22670900 | -2.61220100 | -1.45277400 |

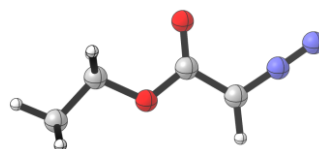
INT1



| | | | |
|---|-------------|-------------|-------------|
| N | 0.31676500 | -0.38349800 | 0.11861000 |
| N | -0.55344800 | 0.60081000 | 0.11764400 |
| C | -1.94369400 | 0.30280600 | 0.17053100 |
| C | 1.60684900 | -0.04163900 | -0.29956900 |
| O | 1.88651000 | 0.88049900 | -1.02781400 |
| O | -2.75085600 | 1.16307900 | 0.39527600 |
| O | -2.17838900 | -0.96425100 | -0.05175900 |
| C | -3.56268500 | -1.37060100 | 0.00528300 |
| H | -4.11863100 | -0.80387100 | -0.75479200 |
| H | -3.95936800 | -1.10203400 | 0.99445400 |
| C | -3.61126500 | -2.85528100 | -0.24360900 |
| H | -4.65527900 | -3.19402200 | -0.20701300 |
| H | -3.19979800 | -3.09853000 | -1.23282100 |
| H | -3.04111900 | -3.39765300 | 0.52308900 |
| C | 3.83281300 | -0.76781200 | -0.24180900 |
| H | 4.16874700 | 0.23472100 | 0.06079900 |
| H | 3.88174600 | -0.82296900 | -1.33923300 |
| O | 2.46516600 | -0.93436300 | 0.16349700 |
| C | 4.64324000 | -1.85637600 | 0.41439300 |
| H | 4.28933100 | -2.84837800 | 0.10105600 |
| H | 5.69719800 | -1.75427600 | 0.12274300 |

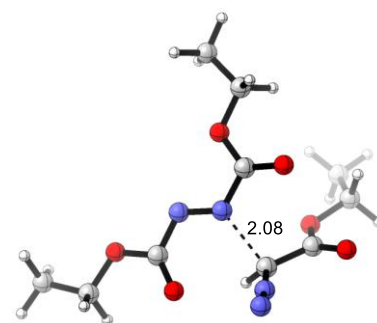
| | | | |
|---|-------------|-------------|-------------|
| H | 4.57604300 | -1.78544700 | 1.50891600 |
| C | -0.57284600 | 2.98486800 | -0.73950700 |
| H | -1.65665600 | 2.95186300 | -0.90387700 |
| H | -0.05159600 | 2.69616400 | -1.66261700 |
| H | -0.26972800 | 3.99377800 | -0.43770300 |
| C | -0.18567800 | 2.00093900 | 0.32230000 |
| N | 0.48229200 | 2.26690400 | 1.34450700 |

10a



| | | | |
|---|-------------|-------------|-------------|
| C | -1.29481200 | -0.80168800 | -0.00014300 |
| C | -0.22218300 | 0.18934900 | -0.00004000 |
| O | -0.37928800 | 1.39492800 | 0.00002400 |
| O | 0.97340300 | -0.42068200 | 0.00003700 |
| C | 2.13667900 | 0.43015000 | 0.00017900 |
| H | 2.10352000 | 1.08094900 | -0.88833100 |
| H | 2.10335200 | 1.08089000 | 0.88872700 |
| N | -2.52309000 | -0.36063200 | -0.00019700 |
| N | -3.58002400 | 0.04507300 | -0.00024600 |
| H | -1.14913500 | -1.88188900 | -0.00017700 |
| C | 3.36009400 | -0.45657000 | 0.00026100 |
| H | 4.26797000 | 0.16663400 | 0.00039400 |
| H | 3.38214800 | -1.09959500 | 0.89431900 |
| H | 3.38234500 | -1.09949900 | -0.89386200 |

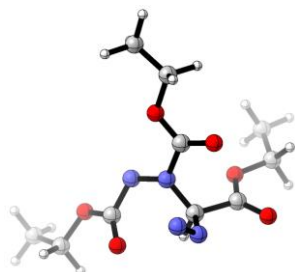
TS2



| | | | |
|---|-------------|-------------|-------------|
| N | -1.29126900 | 0.72653300 | 0.12611400 |
| N | -0.17710000 | 0.16120900 | 0.42655100 |
| C | 0.93995900 | 0.92395900 | 0.77464200 |
| C | -2.39503500 | -0.09826100 | -0.01462100 |
| O | -2.46036600 | -1.28119500 | 0.25371600 |
| O | 1.93849800 | 0.41209100 | 1.22181500 |
| O | 0.78249600 | 2.21947700 | 0.55949600 |
| C | 1.89647900 | 3.05630700 | 0.91192600 |
| H | 2.77767900 | 2.72739100 | 0.34210500 |
| H | 2.11478800 | 2.91869400 | 1.98082300 |
| C | 1.51777000 | 4.47988000 | 0.59177600 |

| | | | |
|---|-------------|-------------|-------------|
| H | 2.35079500 | 5.14733600 | 0.85060700 |
| H | 1.29999100 | 4.59319300 | -0.47934500 |
| H | 0.63324700 | 4.78628700 | 1.16725200 |
| C | -4.65518700 | -0.09222500 | -0.64030500 |
| H | -4.95569800 | -0.52309400 | 0.32641800 |
| H | -4.49376400 | -0.92559200 | -1.34036500 |
| O | -3.42196300 | 0.61406700 | -0.46844500 |
| C | -5.67869800 | 0.88594400 | -1.16035900 |
| H | -5.36036500 | 1.30612100 | -2.12467600 |
| H | -6.63920200 | 0.37283700 | -1.30399500 |
| H | -5.82677100 | 1.70969000 | -0.44812400 |
| C | 0.24554200 | -1.84175500 | 0.05689600 |
| C | 1.73075400 | -1.86727400 | -0.12673400 |
| O | 2.48570500 | -2.49760100 | 0.56149000 |
| O | 2.05821600 | -1.12217000 | -1.16750200 |
| C | 3.46467700 | -0.92145700 | -1.38415700 |
| H | 3.89763700 | -0.53713700 | -0.44930900 |
| H | 3.92911900 | -1.89345400 | -1.60489300 |
| N | -0.18188100 | -2.55539900 | 1.09059900 |
| N | -0.55953500 | -3.03979500 | 2.03221200 |
| H | -0.42033800 | -1.85447300 | -0.80520900 |
| C | 3.61857000 | 0.05278900 | -2.52388400 |
| H | 4.68574000 | 0.22981700 | -2.71391800 |
| H | 3.16225500 | -0.34403700 | -3.44142200 |
| H | 3.14370500 | 1.01378700 | -2.27991900 |

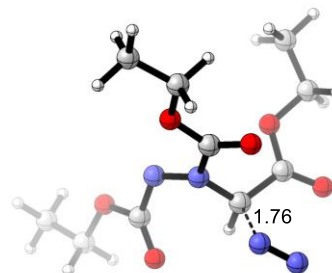
INT2



| | | | |
|---|-------------|-------------|-------------|
| N | 1.11690800 | 0.58458600 | 0.13256400 |
| N | 0.01233000 | 0.12020200 | -0.40635100 |
| C | -1.09987500 | 0.99473300 | -0.55053200 |
| C | 2.29766400 | -0.09072500 | -0.18068900 |
| O | 2.47498900 | -0.78441800 | -1.15601800 |
| O | -2.12117500 | 0.59586400 | -1.04544300 |
| O | -0.85235200 | 2.19777200 | -0.10948100 |
| C | -1.93071400 | 3.15125800 | -0.23394900 |
| H | -2.79981800 | 2.75867400 | 0.31240500 |
| H | -2.19739000 | 3.22971800 | -1.29714700 |
| C | -1.44646300 | 4.46078100 | 0.33045100 |
| H | -2.24769800 | 5.20737000 | 0.24870100 |
| H | -1.17646300 | 4.35279600 | 1.38988700 |
| H | -0.57177400 | 4.82519300 | -0.22551200 |
| C | 4.52508800 | -0.35186400 | 0.49638000 |

| | | | |
|---|-------------|-------------|-------------|
| H | 4.89913900 | 0.00822200 | -0.47323500 |
| H | 4.43315400 | -1.44620100 | 0.43728300 |
| O | 3.22013100 | 0.20683300 | 0.71738400 |
| C | 5.40968400 | 0.07941900 | 1.63808400 |
| H | 5.01531700 | -0.28669600 | 2.59616100 |
| H | 6.41747200 | -0.33329000 | 1.49563700 |
| H | 5.48440300 | 1.17486200 | 1.68065200 |
| C | -0.22358700 | -1.26241800 | -0.80224600 |
| C | -1.52142200 | -1.82783100 | -0.21177800 |
| O | -2.22186400 | -2.61297300 | -0.78021300 |
| O | -1.69066200 | -1.38294700 | 1.01920100 |
| C | -2.88948800 | -1.80511000 | 1.69665700 |
| H | -3.75032800 | -1.52854600 | 1.07103800 |
| H | -2.86926200 | -2.90047300 | 1.78688900 |
| N | -0.26575700 | -1.44807800 | -2.28380300 |
| N | -0.02054000 | -0.60312000 | -3.04535100 |
| H | 0.60460600 | -1.88464800 | -0.44427900 |
| C | -2.92176600 | -1.12348700 | 3.04005700 |
| H | -3.82722100 | -1.42745100 | 3.58223200 |
| H | -2.04510000 | -1.40331200 | 3.64046500 |
| H | -2.93689600 | -0.03093300 | 2.92136700 |

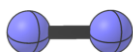
TS3



| | | | |
|---|-------------|-------------|-------------|
| N | 1.17053500 | 0.63169100 | -0.01456900 |
| N | 0.05059900 | 0.11748900 | -0.48005500 |
| C | -1.06714700 | 0.97474900 | -0.67725600 |
| C | 2.34646300 | -0.07682800 | -0.27762100 |
| O | 2.52045100 | -0.83879700 | -1.20020400 |
| O | -2.11855300 | 0.53198200 | -1.05608600 |
| O | -0.78709600 | 2.22476900 | -0.41268100 |
| C | -1.86851500 | 3.16342300 | -0.59058100 |
| H | -2.70395000 | 2.85156300 | 0.05219100 |
| H | -2.20129900 | 3.11134400 | -1.63672500 |
| C | -1.35008400 | 4.52976700 | -0.22587700 |
| H | -2.15423900 | 5.26725000 | -0.35061800 |
| H | -1.01455600 | 4.55260000 | 0.82005100 |
| H | -0.51123700 | 4.81469100 | -0.87566900 |
| C | 4.57401200 | -0.29411500 | 0.41795300 |
| H | 4.94568200 | -0.01592800 | -0.57912900 |
| H | 4.48057000 | -1.38947300 | 0.45008000 |
| O | 3.27037700 | 0.28279800 | 0.59593900 |

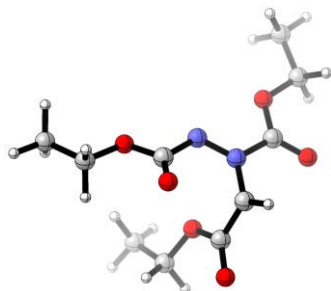
| | | | |
|---|-------------|-------------|-------------|
| C | 5.46217700 | 0.22915600 | 1.51772900 |
| H | 5.07096600 | -0.05719100 | 2.50384800 |
| H | 6.46968000 | -0.19367300 | 1.40643200 |
| H | 5.53664000 | 1.32442100 | 1.47017300 |
| C | -0.21216900 | -1.28613800 | -0.62951700 |
| C | -1.34486900 | -1.83280600 | 0.20279800 |
| O | -1.88794000 | -2.87319900 | -0.05210500 |
| O | -1.62577200 | -1.05315800 | 1.23479900 |
| C | -2.74309700 | -1.44298700 | 2.05244800 |
| H | -3.62626000 | -1.53883700 | 1.40428500 |
| H | -2.53003800 | -2.43034100 | 2.48669900 |
| N | -0.62407100 | -1.46269000 | -2.32923400 |
| N | -1.12440100 | -2.38750400 | -2.74493500 |
| H | 0.69034900 | -1.89566000 | -0.58684700 |
| C | -2.92841000 | -0.38529200 | 3.10994900 |
| H | -3.77751100 | -0.65451100 | 3.75248100 |
| H | -2.03007600 | -0.29927600 | 3.73686600 |
| H | -3.13525700 | 0.59137600 | 2.64999100 |

N₂



| | | | |
|---|------------|------------|-------------|
| N | 0.00000000 | 0.00000000 | 0.54652300 |
| N | 0.00000000 | 0.00000000 | -0.54652300 |

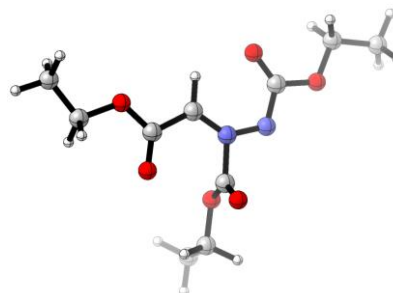
INT3-T



| | | | |
|---|-------------|-------------|-------------|
| N | -0.37038100 | 0.80679400 | -0.38627600 |
| N | -0.97909200 | -0.33812300 | -0.63450700 |
| C | -2.34677000 | -0.47377900 | -0.27882000 |
| C | 0.92980300 | 0.91147800 | -0.87837900 |
| O | 1.39905000 | 0.27811700 | -1.79843200 |
| O | -2.90530700 | -1.53140800 | -0.39378400 |
| O | -2.86330000 | 0.65070400 | 0.15054900 |
| C | -4.25387000 | 0.60119300 | 0.52939700 |
| H | -4.37029400 | -0.15354300 | 1.31997500 |
| H | -4.83853000 | 0.27737000 | -0.34329600 |
| C | -4.64767500 | 1.97813700 | 0.99667900 |
| H | -5.70534600 | 1.97198700 | 1.29233800 |
| H | -4.04465600 | 2.28270200 | 1.86311200 |
| H | -4.51427400 | 2.71541300 | 0.19305100 |

| | | | |
|---|-------------|-------------|-------------|
| C | 2.92104200 | 2.11724900 | -0.62295100 |
| H | 2.91684500 | 2.39789800 | -1.68638800 |
| H | 3.50121400 | 1.18784800 | -0.52250900 |
| O | 1.56944100 | 1.85947300 | -0.21306000 |
| C | 3.46582800 | 3.22001800 | 0.24855700 |
| H | 3.46289000 | 2.92170900 | 1.30622700 |
| H | 4.50011400 | 3.44191700 | -0.04694800 |
| H | 2.86775400 | 4.13514000 | 0.13757100 |
| C | -0.35819000 | -1.51441000 | -1.14727200 |
| C | 0.75230300 | -2.13409300 | -0.43304300 |
| O | 1.33633300 | -3.11411000 | -0.83163100 |
| O | 1.06322900 | -1.47056300 | 0.68336000 |
| C | 2.23087600 | -1.90840900 | 1.39150900 |
| H | 2.06791600 | -2.93907500 | 1.73926700 |
| H | 3.08004100 | -1.91874700 | 0.69191800 |
| H | -0.70098100 | -1.92114800 | -2.09693300 |
| C | 2.45410300 | -0.95158300 | 2.53532700 |
| H | 3.35334600 | -1.24465700 | 3.09361600 |
| H | 2.59278800 | 0.07212500 | 2.15917600 |
| H | 1.59721600 | -0.96013900 | 3.22327800 |

INT3-S

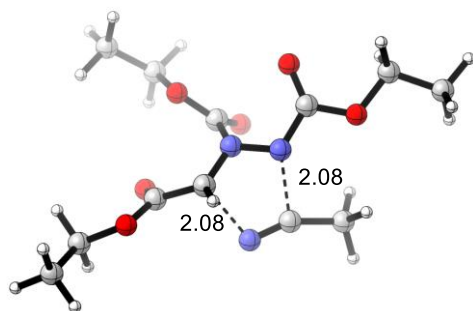


| | | | |
|---|-------------|-------------|-------------|
| N | -1.56463800 | 0.38970000 | 0.30711100 |
| N | -0.26740300 | 0.17180600 | 0.32694000 |
| C | 0.37115700 | 1.46449300 | 0.74377400 |
| C | -2.37823300 | -0.66586700 | -0.02631500 |
| O | -2.05795700 | -1.80520600 | -0.30682400 |
| O | 0.43188900 | 1.76724000 | 1.88725100 |
| O | 0.67590400 | 2.13211800 | -0.32656700 |
| C | 1.34915700 | 3.39581100 | -0.11045500 |
| H | 2.24400300 | 3.19256700 | 0.49445200 |
| H | 0.67495800 | 4.04631200 | 0.46384400 |
| C | 1.68864400 | 3.96833100 | -1.46048600 |
| H | 2.20676600 | 4.92700000 | -1.32461600 |
| H | 2.35033200 | 3.28872100 | -2.01474100 |
| H | 0.77894400 | 4.14397900 | -2.05076400 |
| C | -4.63572400 | -1.23728800 | -0.31974000 |
| H | -4.54573600 | -2.07862400 | 0.38381100 |
| H | -4.44051400 | -1.62811400 | -1.32978700 |
| O | -3.64802500 | -0.25476000 | -0.00056700 |
| C | -5.98912600 | -0.57664600 | -0.22925800 |

| | | | |
|---|-------------|-------------|-------------|
| H | -6.06289800 | 0.25850900 | -0.93991300 |
| H | -6.77424600 | -1.30698600 | -0.46756500 |
| H | -6.16707500 | -0.19240400 | 0.78495000 |
| C | 0.46968300 | -0.87896700 | 0.07959600 |
| C | 1.94282700 | -0.77300700 | 0.18873900 |
| O | 2.54324300 | 0.22230700 | 0.51943600 |
| O | 2.50941000 | -1.92278900 | -0.12639000 |
| C | 3.94644000 | -1.97259700 | -0.06408700 |
| H | 4.34926200 | -1.20569400 | -0.74135200 |
| H | 4.25771400 | -1.71803800 | 0.95937900 |
| H | -0.00766300 | -1.81060100 | -0.20438300 |
| C | 4.37641600 | -3.36174300 | -0.45954200 |
| H | 5.47190300 | -3.42926500 | -0.42042300 |
| H | 3.95632800 | -4.10977800 | 0.22695700 |
| H | 4.04907600 | -3.59452700 | -1.48228800 |

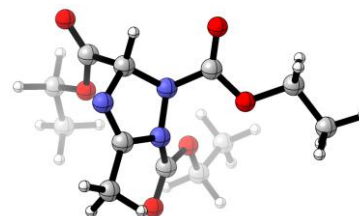
| | | | |
|---|-------------|-------------|-------------|
| O | -2.47752400 | 0.13085500 | -0.95952800 |
| O | -3.21954900 | -1.24056900 | 0.64903800 |
| C | -4.56944000 | -1.10454500 | 0.16446100 |
| H | -4.84545000 | -0.04115600 | 0.20799600 |
| H | -4.58994500 | -1.41844100 | -0.88905100 |
| H | -0.84568500 | -1.66501200 | 1.31760800 |
| C | -5.45851200 | -1.95839000 | 1.03078300 |
| H | -6.49646300 | -1.87302700 | 0.68222700 |
| H | -5.15799000 | -3.01382400 | 0.97605300 |
| H | -5.41440600 | -1.62950200 | 2.07823800 |
| C | 2.24126100 | -2.45235000 | -1.37975800 |
| H | 2.68157800 | -1.57156300 | -1.86485200 |
| H | 2.17588500 | -3.28248500 | -2.09461500 |
| H | 2.87894900 | -2.72430800 | -0.53052900 |
| C | 0.89465900 | -2.11946300 | -0.89585000 |
| N | -0.28186700 | -2.24229200 | -0.88573900 |

TS4



| | | | |
|---|-------------|-------------|-------------|
| N | 1.27267800 | -0.64809500 | 0.52901000 |
| N | 0.07426600 | -0.04945900 | 0.43086400 |
| C | -0.04322800 | 1.12713600 | -0.44505600 |
| C | 2.32471300 | 0.22556000 | 0.66071700 |
| O | 2.24631200 | 1.41738900 | 0.87822400 |
| O | 0.51946400 | 1.18420000 | -1.49246100 |
| O | -0.81376200 | 2.01141400 | 0.12410100 |
| C | -1.19756100 | 3.13299400 | -0.69657200 |
| H | -1.62460000 | 2.73460300 | -1.62800300 |
| H | -0.29062000 | 3.70300500 | -0.94281100 |
| C | -2.19425200 | 3.95033800 | 0.08240300 |
| H | -2.50208300 | 4.81695600 | -0.51777500 |
| H | -3.08615700 | 3.35219300 | 0.31575000 |
| H | -1.75301800 | 4.31447000 | 1.02042400 |
| C | 4.67058200 | 0.35324500 | 0.64193100 |
| H | 4.69875100 | 0.82517600 | 1.63528100 |
| H | 4.63738200 | 1.15697800 | -0.10823700 |
| O | 3.47942000 | -0.43248500 | 0.53555300 |
| C | 5.84785900 | -0.56492700 | 0.42584300 |
| H | 5.80465900 | -1.02537000 | -0.57145700 |
| H | 6.78218300 | 0.00733900 | 0.50407100 |
| H | 5.86375900 | -1.36243700 | 1.18198300 |
| C | -0.93524200 | -0.89324600 | 0.55517900 |
| C | -2.28869800 | -0.57820100 | -0.00585700 |

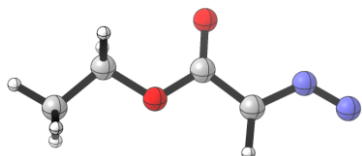
11a



| | | | |
|---|-------------|-------------|-------------|
| C | -0.90101900 | 1.88909900 | -0.30683300 |
| C | -2.14526100 | 1.27318200 | -0.95589500 |
| O | -2.87596200 | 1.84618400 | -1.71565600 |
| O | -2.31258100 | 0.02982300 | -0.52722100 |
| C | -3.44675600 | -0.70343600 | -1.01405400 |
| H | -4.35998600 | -0.23687000 | -0.61583100 |
| H | -3.47331700 | -0.62341600 | -2.10995800 |
| H | -0.61280200 | 2.79017100 | -0.85914400 |
| C | -3.28941200 | -2.13065700 | -0.55306100 |
| H | -4.15452800 | -2.72409800 | -0.87822800 |
| H | -2.37989200 | -2.57455800 | -0.98195600 |
| H | -3.22421500 | -2.17926100 | 0.54341700 |
| C | -0.78010900 | 1.01701400 | 3.24553600 |
| H | -1.27434400 | 1.89512000 | 3.67525300 |
| H | 0.20512500 | 0.86455600 | 3.70438500 |
| H | -1.38148100 | 0.11988500 | 3.44363000 |
| C | -0.64711800 | 1.21690900 | 1.77909500 |
| N | -1.20995900 | 2.13460900 | 1.09767800 |
| N | 0.20809900 | 0.93835100 | -0.27804200 |
| N | 0.16469200 | 0.35850600 | 0.99066000 |
| C | 0.19246400 | -1.02993600 | 1.13495900 |
| C | 1.43996100 | 1.30299800 | -0.81277600 |
| O | 1.53780900 | 2.06823600 | -1.73856100 |
| O | -0.05972000 | -1.58383500 | 2.17420100 |
| O | 0.57220000 | -1.61992900 | 0.01825800 |

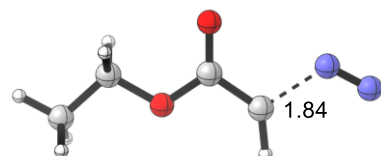
| | | | |
|---|-------------|-------------|-------------|
| C | 0.71856300 | -3.04801800 | 0.07670600 |
| H | -0.24195400 | -3.48937100 | 0.37846200 |
| H | 1.46186500 | -3.29117900 | 0.84968200 |
| C | 1.15239900 | -3.51629300 | -1.28886700 |
| H | 1.28128900 | -4.60694400 | -1.27874300 |
| H | 0.39899600 | -3.26078400 | -2.04711700 |
| H | 2.10867500 | -3.05433900 | -1.57190100 |
| C | 3.74474000 | 0.88293500 | -0.77760300 |
| H | 3.98851400 | 1.95225200 | -0.70076600 |
| H | 3.72106200 | 0.61538900 | -1.84380100 |
| O | 2.43737900 | 0.66768700 | -0.22275500 |
| C | 4.71379800 | 0.02664200 | -0.00291600 |
| H | 4.44864500 | -1.03635800 | -0.09119600 |
| H | 5.72783600 | 0.16757200 | -0.40056600 |
| H | 4.71420300 | 0.30400600 | 1.06040900 |

10a-T



| | | | |
|---|-------------|-------------|-------------|
| C | 1.45981800 | 0.14671200 | 0.00000000 |
| C | 0.00000000 | 0.36509400 | 0.00000000 |
| O | -0.52398100 | 1.45031600 | 0.00000000 |
| O | -0.64790700 | -0.79304600 | 0.00000000 |
| C | -2.08231600 | -0.72279300 | 0.00000000 |
| H | -2.40457900 | -0.16010600 | 0.88854500 |
| H | -2.40457900 | -0.16010600 | -0.88854500 |
| N | 2.25782100 | 1.25835400 | 0.00000000 |
| N | 3.45534500 | 1.23304500 | 0.00000000 |
| H | 1.89751600 | -0.85500400 | 0.00000000 |
| C | -2.61612100 | -2.13259500 | 0.00000000 |
| H | -3.71419400 | -2.10834700 | 0.00000000 |
| H | -2.27975000 | -2.67644600 | -0.89365000 |
| H | -2.27975000 | -2.67644600 | 0.89365000 |

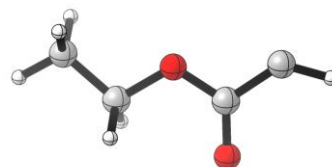
TS5



| | | | |
|---|-------------|-------------|-------------|
| C | 1.42842600 | -0.02196700 | 0.00000000 |
| C | 0.00000000 | 0.24745300 | 0.00000000 |
| O | -0.48875200 | 1.35353800 | 0.00000000 |
| O | -0.71118300 | -0.88320500 | 0.00000000 |
| C | -2.13852400 | -0.73770700 | 0.00000000 |
| H | -2.43453600 | -0.15972500 | 0.88814500 |
| H | -2.43453600 | -0.15972500 | -0.88814500 |

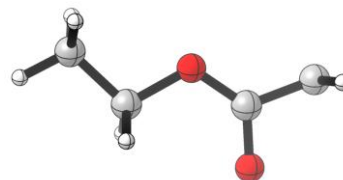
| | | | |
|---|-------------|-------------|-------------|
| N | 2.43596400 | 1.51861100 | 0.00000000 |
| N | 3.55493000 | 1.44046700 | 0.00000000 |
| H | 1.96543700 | -0.97151400 | 0.00000000 |
| C | -2.74390800 | -2.11878700 | 0.00000000 |
| H | -3.83957700 | -2.04060100 | 0.00000000 |
| H | -2.43476300 | -2.67929500 | -0.89330900 |
| H | -2.43476300 | -2.67929500 | 0.89330900 |

INT4-T



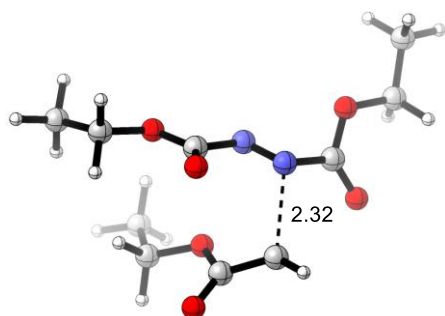
| | | | |
|---|-------------|-------------|-------------|
| C | 2.13802200 | -1.01949300 | 0.00014600 |
| C | 1.11716400 | 0.00182600 | -0.00067400 |
| O | 1.36662900 | 1.18870300 | 0.00040900 |
| O | -0.11886700 | -0.49819800 | -0.00042900 |
| C | -1.19083000 | 0.45321100 | -0.00001300 |
| H | -1.09513300 | 1.09598500 | 0.88795100 |
| H | -1.09560600 | 1.09621100 | -0.88786500 |
| H | 3.22490100 | -0.93779000 | 0.00098800 |
| C | -2.48959600 | -0.31366800 | 0.00023800 |
| H | -3.33358400 | 0.38930700 | 0.00055200 |
| H | -2.56585600 | -0.94939300 | -0.89301100 |
| H | -2.56537900 | -0.94962000 | 0.89336500 |

INT4-S



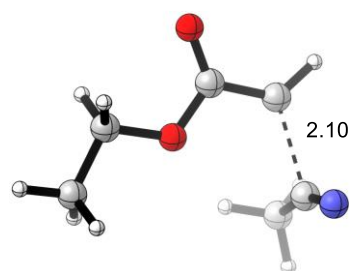
| | | | |
|---|-------------|-------------|-------------|
| C | -2.25758800 | -0.86466100 | -0.15015900 |
| C | -1.07776400 | -0.06605900 | -0.01124500 |
| O | -1.43692500 | 1.10102700 | -0.00417000 |
| O | 0.14502800 | -0.52212500 | -0.00220500 |
| C | 1.20381900 | 0.46510000 | 0.02239700 |
| H | 1.08300700 | 1.12260300 | -0.84978300 |
| H | 1.09081100 | 1.07150900 | 0.93187700 |
| H | -2.69770400 | -1.01944900 | 0.85234900 |
| C | 2.51571400 | -0.27467900 | -0.00340200 |
| H | 3.34142500 | 0.44924900 | 0.01753500 |
| H | 2.60815000 | -0.93449700 | 0.87030600 |
| H | 2.60439900 | -0.87883300 | -0.91682700 |

TS6



| | | | |
|---|-------------|-------------|-------------|
| C | 0.11004100 | 2.31665000 | -0.84628600 |
| C | -1.23188800 | 2.16959900 | -0.33738000 |
| O | -2.20515300 | 2.72878600 | -0.79418800 |
| O | -1.28222600 | 1.32217200 | 0.70125000 |
| C | -2.57134700 | 1.04368500 | 1.25950900 |
| H | -3.06472200 | 1.99392800 | 1.51070600 |
| H | -3.18792700 | 0.54308300 | 0.49492300 |
| H | 0.48223100 | 2.93210700 | -1.66319400 |
| C | -2.36028200 | 0.17720200 | 2.47659800 |
| H | -3.33028900 | -0.08313600 | 2.92185600 |
| H | -1.83625800 | -0.74878100 | 2.20122000 |
| H | -1.76341700 | 0.71100600 | 3.22958800 |
| N | 0.48802200 | -0.62943700 | -0.19461100 |
| N | 1.16683100 | 0.24938100 | -0.73362800 |
| C | 2.40859200 | 0.52991100 | -0.04951800 |
| C | -0.75911500 | -0.85180200 | -0.91632400 |
| O | -1.04492200 | -0.34494400 | -1.96213200 |
| O | 2.66814600 | 1.62280600 | 0.36032100 |
| O | 3.17536400 | -0.53260600 | -0.03527100 |
| C | 4.49037300 | -0.36748500 | 0.54013000 |
| H | 4.36816100 | -0.08022600 | 1.59398100 |
| H | 4.99341100 | 0.45607600 | 0.01409500 |
| C | 5.22366100 | -1.67420600 | 0.38796000 |
| H | 6.22859800 | -1.57749000 | 0.82030700 |
| H | 4.69454000 | -2.48167400 | 0.91241700 |
| H | 5.32445900 | -1.94329000 | -0.67247500 |
| C | -2.76189300 | -2.06026800 | -0.78790300 |
| H | -2.56652800 | -2.68306700 | -1.67336400 |
| H | -3.27511500 | -1.14748300 | -1.12177200 |
| O | -1.48973800 | -1.69038400 | -0.21981900 |
| C | -3.54412800 | -2.80118600 | 0.26512000 |
| H | -3.75003300 | -2.15298800 | 1.12848900 |
| H | -4.50257700 | -3.12837300 | -0.15986500 |
| H | -2.99435600 | -3.68855400 | 0.60803900 |

TS7



| | | | |
|---|-------------|-------------|-------------|
| C | 1.11363100 | 1.27439900 | -0.15893200 |
| C | -0.32967100 | 1.18838800 | -0.09496100 |
| O | -1.05533300 | 2.15956500 | -0.11037900 |
| O | -0.77679800 | -0.06848900 | -0.00721000 |
| C | -2.19780300 | -0.23792600 | 0.07747100 |
| H | -2.56478000 | 0.29877500 | 0.96492200 |
| H | -2.66299800 | 0.22199500 | -0.80701700 |
| H | 1.71501000 | 2.16808700 | -0.32645800 |
| C | -2.48330600 | -1.71654900 | 0.15815500 |
| H | -3.56711000 | -1.87893900 | 0.23258100 |
| H | -2.11523500 | -2.23472800 | -0.73865000 |
| H | -2.00348400 | -2.15747900 | 1.04310600 |
| C | 2.08845900 | -1.11308000 | -1.07193900 |
| H | 2.56283500 | -0.46223200 | -1.81750300 |
| H | 1.03381600 | -1.25527900 | -1.33803100 |
| H | 2.60443200 | -2.08145000 | -1.03707300 |
| C | 2.17485900 | -0.48528000 | 0.26325700 |
| N | 2.49393600 | -0.40100900 | 1.38950300 |

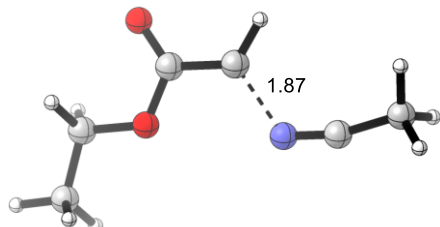
INT5



| | | | |
|---|-------------|-------------|-------------|
| C | 1.30917100 | 0.91574300 | -0.00022200 |
| C | -0.14996500 | 1.09075400 | 0.00007500 |
| O | -0.67053400 | 2.18273400 | -0.00006300 |
| O | -0.83786700 | -0.05027400 | 0.00051600 |
| C | -2.26738100 | 0.06150300 | 0.00050400 |
| H | -2.57628900 | 0.63158400 | 0.88910000 |
| H | -2.57617100 | 0.63328500 | -0.88701400 |
| H | 1.87731000 | 1.84663600 | -0.00064500 |
| C | -2.83958500 | -1.33383500 | -0.00082100 |
| H | -3.93675200 | -1.28142700 | -0.00071800 |
| H | -2.51817300 | -1.88641300 | -0.89494900 |
| H | -2.51811000 | -1.88814100 | 0.89221400 |
| C | 1.43224200 | -1.69110700 | 0.00053600 |
| H | 0.80108900 | -1.82426500 | -0.88678800 |
| H | 0.80104500 | -1.82351000 | 0.88791200 |

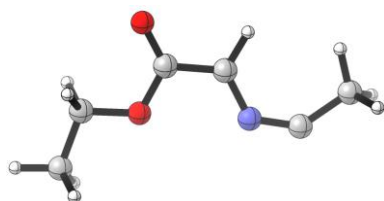
| | | | |
|---|------------|-------------|-------------|
| H | 2.23505500 | -2.43837000 | 0.00079200 |
| C | 2.04392400 | -0.30648000 | -0.00008600 |
| N | 3.32968200 | -0.20693200 | -0.00049100 |

TS8



| | | | |
|---|-------------|-------------|-------------|
| C | -0.80326500 | 0.94777200 | -0.22111900 |
| C | 0.63281200 | 1.01241000 | -0.05088200 |
| O | 1.24314100 | 2.04443300 | 0.15078600 |
| O | 1.23027900 | -0.18235800 | -0.12617100 |
| C | 2.64727900 | -0.19453900 | 0.06094100 |
| H | 3.11545900 | 0.45448800 | -0.69477100 |
| H | 2.88239600 | 0.22933000 | 1.04914900 |
| H | -1.42787800 | 1.83776100 | -0.31724400 |
| C | 3.11793300 | -1.62299700 | -0.06059800 |
| H | 4.20632800 | -1.66922400 | 0.08087000 |
| H | 2.64025800 | -2.25540500 | 0.70095200 |
| H | 2.87815300 | -2.02796300 | -1.05387600 |
| C | -4.23054300 | -0.41119900 | -0.08720100 |
| H | -4.79675000 | -0.51396300 | 0.84785400 |
| H | -4.63921800 | -1.11757400 | -0.82173600 |
| H | -4.33794400 | 0.61619200 | -0.46897400 |
| C | -2.82483000 | -0.70986000 | 0.15365400 |
| N | -1.64921200 | -0.65425200 | 0.24458400 |

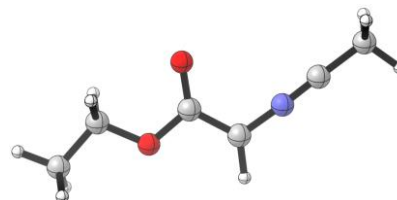
INT6



| | | | |
|---|-------------|-------------|-------------|
| C | -0.99748900 | 0.59835400 | 0.00003400 |
| C | 0.44274400 | 0.87597800 | -0.00004000 |
| O | 0.88603000 | 2.00395900 | 0.00020100 |
| O | 1.20466500 | -0.21719200 | -0.00035500 |
| C | 2.61948200 | -0.00107900 | -0.00037600 |
| H | 2.88976600 | 0.59029700 | -0.88818800 |
| H | 2.88962200 | 0.59157800 | 0.88660600 |
| H | -1.65597500 | 1.47445300 | 0.00043100 |
| C | 3.29411100 | -1.35028700 | 0.00064100 |
| H | 4.38470400 | -1.21879900 | 0.00033900 |
| H | 3.01262500 | -1.92503100 | 0.89414100 |
| H | 3.01232000 | -1.92652500 | -0.89180000 |

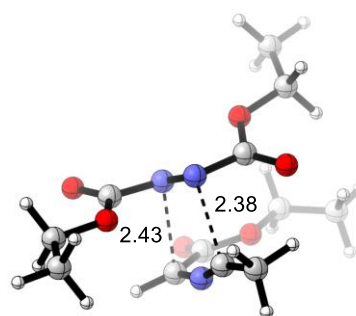
| | | | |
|---|-------------|-------------|-------------|
| C | -3.99070200 | -0.28663400 | 0.00044500 |
| H | -4.56698500 | -0.57363300 | 0.89266700 |
| H | -4.57891900 | -0.59020800 | -0.87824200 |
| H | -3.86182300 | 0.80813900 | -0.01041800 |
| C | -2.69222200 | -0.98837100 | -0.00074000 |
| N | -1.47234800 | -0.65888100 | -0.00058400 |

INT7



| | | | |
|---|-------------|-------------|-------------|
| C | -0.60743000 | -0.94775600 | 0.00010500 |
| C | 0.38439600 | 0.07825200 | 0.00016200 |
| O | 0.18537400 | 1.28284800 | 0.00006200 |
| O | 1.63861600 | -0.44013200 | 0.00036800 |
| C | 2.70458700 | 0.50123200 | 0.00011800 |
| H | 2.62303400 | 1.15120500 | -0.88519800 |
| H | 2.62367600 | 1.15095700 | 0.88568200 |
| H | -0.39533400 | -2.01298200 | 0.00011200 |
| C | 4.00384900 | -0.26909400 | -0.00042800 |
| H | 4.85431800 | 0.42662300 | -0.00059000 |
| H | 4.07686000 | -0.90771200 | 0.89152400 |
| H | 4.07628000 | -0.90743400 | -0.89262700 |
| C | -4.35421600 | 0.30260900 | -0.00017500 |
| H | -5.00359500 | -0.58432400 | 0.00045700 |
| H | -4.56089200 | 0.89494300 | -0.90158900 |
| H | -4.56055000 | 0.89585000 | 0.90071500 |
| C | -2.98009700 | -0.16154000 | -0.00011800 |
| N | -1.89032100 | -0.55301100 | 0.00001400 |

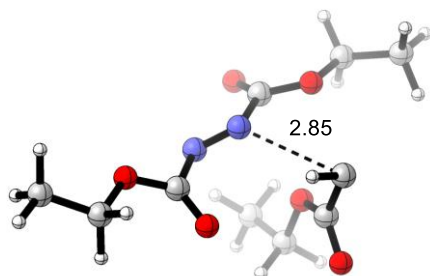
TS9



| | | | |
|---|-------------|-------------|-------------|
| C | -0.85050200 | -1.78367800 | -0.49918900 |
| C | 0.49862800 | -1.90470200 | -1.04083000 |
| O | 0.75648900 | -2.21676800 | -2.17954900 |
| O | 1.42323800 | -1.57834500 | -0.12254100 |
| C | 2.78980200 | -1.54287800 | -0.53765900 |
| H | 2.97479100 | -2.36382000 | -1.24374200 |
| H | 2.96457700 | -0.59396500 | -1.07151700 |

| | | | | | | | |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -1.71535500 | -2.09538100 | -1.08261300 | C | -1.23413700 | -0.83728500 | -2.05609300 |
| C | 3.64673100 | -1.66410700 | 0.70041300 | C | -1.09410700 | -1.73143100 | -0.93026300 |
| H | 4.70730700 | -1.55042100 | 0.43654300 | O | -0.89930500 | -2.88175700 | -1.26878800 |
| H | 3.37964400 | -0.88997800 | 1.43398700 | O | -1.27722600 | -1.30086200 | 0.30280200 |
| H | 3.50613200 | -2.64819100 | 1.16966600 | C | -1.05288300 | -2.24523200 | 1.36995700 |
| C | -1.05410700 | -0.55978700 | 3.18667700 | H | -1.83454300 | -3.01675300 | 1.32544900 |
| H | -1.37679600 | -1.44095100 | 3.75741500 | H | -0.07952800 | -2.72881200 | 1.20497500 |
| H | -1.74593100 | 0.27916000 | 3.34007500 | H | -0.21855400 | -0.57520700 | -2.40127000 |
| H | -0.04972700 | -0.24166400 | 3.49514400 | C | -1.08682900 | -1.47162200 | 2.66363600 |
| C | -0.99296700 | -0.86770900 | 1.76932900 | H | -0.90239700 | -2.15427100 | 3.50416400 |
| N | -1.00218500 | -1.51288300 | 0.78954200 | H | -0.31138700 | -0.69210400 | 2.66590800 |
| N | -0.54403100 | 0.61606400 | -0.75667000 | H | -2.06691900 | -0.99588400 | 2.80915100 |
| N | -0.38646900 | 1.00372300 | 0.43450200 | N | 1.01853900 | 0.73533000 | 0.50538400 |
| C | 0.98619000 | 1.14300600 | 0.81307700 | N | 0.10316100 | 0.94915300 | -0.27758800 |
| C | -1.90541000 | 0.65243900 | -1.20906400 | C | -1.09239500 | 1.48205400 | 0.38669000 |
| O | -2.15982600 | 0.69910100 | -2.38193900 | C | 2.12658700 | 0.06126900 | -0.13638000 |
| O | 1.35678300 | 0.94923000 | 1.94242200 | O | 1.98710700 | -0.96740000 | -0.73302600 |
| O | 1.74209400 | 1.61939500 | -0.16020600 | O | -1.13969800 | 1.90291000 | 1.50094100 |
| C | 3.08298700 | 1.99912000 | 0.18954800 | O | -2.06687700 | 1.38396800 | -0.48283000 |
| H | 3.61997600 | 1.11538900 | 0.56181700 | C | -3.39414600 | 1.68595700 | -0.01137800 |
| H | 3.03351000 | 2.73275900 | 1.00769300 | H | -3.42124900 | 2.74608900 | 0.27875500 |
| C | 3.73353200 | 2.57190000 | -1.04409300 | H | -3.58157800 | 1.07757100 | 0.88557400 |
| H | 4.75974300 | 2.88284000 | -0.80599700 | C | -4.35855100 | 1.37106000 | -1.12467900 |
| H | 3.77464000 | 1.82353900 | -1.84823900 | H | -5.38111300 | 1.59740600 | -0.79424500 |
| H | 3.17786100 | 3.44818400 | -1.40577200 | H | -4.13706300 | 1.97572500 | -2.01494800 |
| C | -4.17880600 | 0.61304300 | -0.63692400 | H | -4.30358400 | 0.30730400 | -1.39432000 |
| H | -4.33978700 | -0.25264200 | -1.29676800 | C | 4.45051100 | 0.13694100 | -0.42371300 |
| H | -4.38794500 | 1.52296600 | -1.21809000 | H | 4.33532100 | 0.05610900 | -1.51369900 |
| O | -2.80146000 | 0.63149100 | -0.23552600 | H | 4.56358600 | -0.87552000 | -0.01158300 |
| C | -5.01948900 | 0.53459200 | 0.61223600 | O | 3.23479200 | 0.70460200 | 0.11643100 |
| H | -4.83629600 | 1.40385500 | 1.25923600 | C | 5.59013400 | 1.04179200 | -0.03660300 |
| H | -6.08356800 | 0.52057200 | 0.34040000 | H | 5.67770500 | 1.11343200 | 1.05616000 |
| H | -4.79205200 | -0.38084200 | 1.17672400 | H | 6.52756100 | 0.63159000 | -0.43534300 |
| | | | | H | 5.44638700 | 2.04923200 | -0.45057900 |

TS10



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