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# Theoretical Prediction of a Base-Catalyzed Bicyclic Boulton-Katritzky Rearrangement

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# Supporting Information

Name: 4-Nitroso-benzo[c]isoxazole (conformer A)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -529.1147135 a.u.

ZPE: 63.675 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | 1.104669 | -0.490081 | 0.000000 |
| C | 0.000000 | 0.414052 | 0.000000 |
| C | -1.332249 | -0.116742 | 0.000000 |
| C | -1.562567 | -1.523624 | 0.000000 |
| C | -0.477186 | -2.353306 | 0.000000 |
| C | 0.852538 | -1.839865 | 0.000000 |
| N | -2.246311 | 0.838826 | 0.000000 |
| O | -1.513646 | 2.019514 | 0.000000 |
| C | -0.199427 | 1.766966 | 0.000000 |
| N | 2.469760 | -0.107081 | 0.000000 |
| O | 2.658600 | 1.100656 | 0.000000 |
| H | -2.575297 | -1.905518 | 0.000000 |
| H | 1.699859 | -2.514497 | 0.000000 |
| H | -0.620549 | -3.426477 | 0.000000 |
| H | 0.457548 | 2.618522 | 0.000000 |

Name: 4-Nitroso-benzo[*c*]isoxazole (conformer B)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -529.1087318 a.u.

ZPE: 63.380 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | -0.021145 | 1.946568 | 0.000000 |
| C | 0.000000 | 0.578002 | 0.000000 |
| C | -1.390393 | 0.226111 | 0.000000 |
| N | -2.172088 | 1.295216 | 0.000000 |
| O | -1.288237 | 2.368595 | 0.000000 |
| C | -1.787281 | -1.140072 | 0.000000 |
| C | -0.805741 | -2.094559 | 0.000000 |
| C | 0.576623 | -1.756837 | 0.000000 |
| C | 0.987922 | -0.447875 | 0.000000 |
| N | 2.359881 | -0.024805 | 0.000000 |
| O | 3.185042 | -0.917061 | 0.000000 |
| H | -2.837271 | -1.402300 | 0.000000 |
| H | 1.328646 | -2.535739 | 0.000000 |
| H | -1.081761 | -3.141947 | 0.000000 |
| H | 0.741482 | 2.706817 | 0.000000 |

Name: 4-Nitroso-benzo[*c*]isoxazole transition state

Level: B3-LYP/6-311+G(2d,p)

Total energy: -529.0410262 a.u.

ZPE: 61.662 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | 0.000000 | 0.374006 | 0.000000 |
| C | 1.227404 | -0.355561 | 0.000000 |
| C | 1.217769 | -1.749477 | 0.000000 |
| C | -0.000001 | -2.435992 | 0.000000 |
| C | -1.217771 | -1.749475 | 0.000000 |
| C | -1.227405 | -0.355559 | 0.000000 |
| N | 2.324496 | 0.443754 | 0.000000 |
| O | 1.977603 | 1.658527 | 0.000000 |
| N | -2.324495 | 0.443754 | 0.000000 |
| C | 0.000002 | 1.701065 | 0.000000 |
| O | -1.977602 | 1.658528 | 0.000000 |
| H | 2.158817 | -2.286247 | 0.000000 |
| H | -2.158818 | -2.286243 | 0.000000 |
| H | -0.000001 | -3.517797 | 0.000000 |
| H | 0.000001 | 2.767258 | 0.000000 |

Name: 4-Nitroso-benzo[*c*]isoxazole anion (conformer A)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -528.5225234 a.u.

ZPE: 54.292 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | -1.119388 | 0.265351 | -0.000031 |
| C | 0.092077 | -0.474213 | -0.000042 |
| C | 1.336117 | 0.268888 | 0.000051 |
| C | 1.334453 | 1.693064 | -0.000075 |
| C | 0.134526 | 2.360384 | 0.000021 |
| C | -1.089189 | 1.654481 | 0.000082 |
| N | 2.395763 | -0.506104 | 0.000068 |
| O | 1.775828 | -1.846929 | -0.000379 |
| C | 0.439775 | -1.851583 | 0.000710 |
| N | -2.461460 | -0.222039 | -0.000008 |
| O | -2.609520 | -1.435450 | -0.000200 |
| H | 2.275093 | 2.233185 | -0.000328 |
| H | -2.036824 | 2.178998 | 0.000318 |
| H | 0.120924 | 3.445617 | -0.000070 |

Name: 4-Nitroso-benzo[*c*]isoxazole anion (conformer B)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -528.5219683 a.u.

ZPE: 54.088 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | 0.066605 | 2.050111 | 0.000000 |
| C | 0.000000 | 0.629005 | 0.000000 |
| C | -1.402537 | 0.271864 | 0.000000 |
| N | -2.195347 | 1.319858 | 0.000000 |
| O | -1.208250 | 2.429435 | 0.000000 |
| C | -1.777106 | -1.099810 | 0.000000 |
| C | -0.792246 | -2.064201 | 0.000000 |
| C | 0.577698 | -1.733625 | 0.000000 |
| C | 0.970593 | -0.401218 | 0.000000 |
| N | 2.350145 | -0.015657 | 0.000000 |
| O | 3.161400 | -0.935616 | 0.000000 |
| H | -2.825664 | -1.376809 | 0.000000 |
| H | 1.337024 | -2.504004 | 0.000000 |
| H | -1.078191 | -3.111912 | 0.000000 |

Name: 4-Nitroso-benzo[*c*]isoxazole anion transition state

Level: B3-LYP/6-311+G(2d,p)

Total energy: -528.4706019 a.u.

ZPE: 53.389 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | 0.000000 | 1.225700 | 0.285216 |
| C | 0.000000 | 1.205700 | 1.675616 |
| C | 0.000000 | 0.000000 | 2.380216 |
| C | 0.000000 | -1.205700 | 1.675616 |
| C | 0.000000 | -1.225700 | 0.285216 |
| C | 0.000000 | 0.000000 | -0.504984 |
| N | 0.000000 | -2.409900 | -0.381684 |
| O | 0.000000 | -2.232900 | -1.631284 |
| C | 0.000000 | 0.000000 | -1.865184 |
| N | 0.000000 | 2.409900 | -0.381684 |
| O | 0.000000 | 2.232900 | -1.631284 |
| H | 0.000000 | 2.157800 | 2.195116 |
| H | 0.000000 | -2.157800 | 2.195116 |
| H | 0.000000 | 0.000000 | 3.463616 |

Name: 5-Dimethylamino-4-nitroso-benzo[*c*]isoxazole anion (conformer A)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -662.5153790 a.u.

ZPE: 99.477 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | 0.876087 | -0.391466 | -0.032297 |
| C | 0.317294 | -1.705943 | -0.013582 |
| C | -1.029096 | -1.955044 | 0.033623 |
| C | -1.932932 | -0.859254 | 0.050894 |
| C | -1.414291 | 0.477285 | -0.025624 |
| C | -0.010654 | 0.710595 | -0.094341 |
| C | 2.913379 | 0.261508 | 1.148277 |
| C | 3.061985 | -1.264400 | -0.715248 |
| C | -2.525738 | 1.354963 | 0.008335 |
| N | 2.278642 | -0.232108 | -0.065887 |
| N | 0.395856 | 2.001627 | -0.483342 |
| N | -3.245943 | -0.899525 | 0.125122 |
| O | 1.549059 | 2.347842 | -0.210551 |
| O | -3.580030 | 0.535987 | 0.091669 |
| H | 0.998349 | -2.548933 | -0.002996 |
| H | -1.398435 | -2.974281 | 0.075230 |
| H | 3.908011 | 0.650354 | 0.910496 |
| H | 2.327981 | 1.072843 | 1.568245 |
| H | 3.022333 | -0.539072 | 1.901344 |
| H | 2.586592 | -1.565954 | -1.648585 |
| H | 4.051157 | -0.859523 | -0.949165 |
| H | 3.215679 | -2.165501 | -0.094983 |

Name: 5-Dimethylamino-4-nitroso-benzo[*c*]isoxazole anion (conformer B)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -662.5152080 a.u.

ZPE: 99.399 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | 1.004040 | -0.422070 | -0.032835 |
| C | 0.526663 | -1.771674 | -0.009523 |
| C | -0.805342 | -2.074923 | 0.023187 |
| C | -1.761072 | -1.025530 | 0.045117 |
| C | -1.335686 | 0.347607 | 0.017650 |
| C | 0.066332 | 0.637589 | -0.068202 |
| C | 3.009757 | 0.810045 | 0.813844 |
| C | 3.293862 | -1.216578 | -0.494892 |
| C | -2.515002 | 1.135151 | 0.053011 |
| N | 2.382033 | -0.208120 | -0.008498 |
| N | 0.645762 | 1.892089 | -0.315537 |
| N | -3.068880 | -1.166703 | 0.096410 |
| O | -0.107114 | 2.870038 | -0.323503 |
| O | -3.507551 | 0.225008 | 0.101045 |
| H | 1.247042 | -2.579128 | 0.026498 |
| H | -1.132283 | -3.108953 | 0.060982 |
| H | 3.502843 | 1.579498 | 0.210882 |
| H | 2.267037 | 1.305330 | 1.431896 |
| H | 3.761359 | 0.341581 | 1.469101 |
| H | 2.851711 | -1.771296 | -1.321792 |
| H | 4.199624 | -0.729110 | -0.869828 |
| H | 3.606272 | -1.936849 | 0.281155 |

Name: 5-Dimethylamino-4-nitroso-benzo[*c*]isoxazole anion (transition state)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -662.4735208 a.u.

ZPE: 98.849 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | 1.081220 | -0.384106 | -0.043077 |
| C | 0.593623 | -1.718883 | -0.003596 |
| C | 0.125695 | 0.677750 | -0.054386 |
| C | -0.761753 | -1.997487 | 0.041096 |
| C | -1.709127 | -0.981101 | 0.049067 |
| C | -1.313833 | 0.411988 | 0.004729 |
| C | 3.117473 | 0.946613 | 0.534556 |
| C | 3.337252 | -1.313568 | -0.301225 |
| C | -2.271655 | 1.388929 | -0.014957 |
| N | 2.452615 | -0.181500 | -0.108844 |
| N | 0.501145 | 1.967634 | -0.180958 |
| N | -3.030734 | -1.249403 | 0.089424 |
| O | -0.486531 | 2.762052 | -0.199063 |
| O | -3.700526 | -0.168299 | 0.076434 |
| H | 1.288448 | -2.543898 | 0.034614 |
| H | -1.107365 | -3.024706 | 0.086477 |
| H | 3.964434 | 1.269036 | -0.079005 |
| H | 2.428382 | 1.777359 | 0.629979 |
| H | 3.503976 | 0.652412 | 1.523278 |
| H | 2.971445 | -1.965495 | -1.094407 |
| H | 4.316654 | -0.935288 | -0.600600 |
| H | 3.475927 | -1.917366 | 0.610091 |

Name: 7-Dimethylamino-4-nitroso-benzo[*c*]isoxazole anion (conformer A)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -662.5321762 a.u.

ZPE: 100.061 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | 0.209150 | 0.708967 | -0.061477 |
| C | -1.218969 | 0.494727 | -0.017571 |
| C | -1.716978 | -0.840408 | 0.035395 |
| C | -0.807831 | -1.887593 | 0.041054 |
| C | 0.579845 | -1.679623 | 0.005456 |
| C | 1.136855 | -0.403946 | -0.048485 |
| C | 3.364783 | -1.376700 | -0.263981 |
| C | 3.154072 | 0.918868 | 0.501217 |
| C | -1.827524 | 1.773539 | -0.078304 |
| N | 2.510100 | -0.214211 | -0.155161 |
| N | 0.521026 | 1.985481 | -0.146317 |
| N | -3.049633 | -1.302330 | 0.088551 |
| O | -0.797713 | 2.623654 | -0.150134 |
| O | -3.942595 | -0.456656 | 0.099279 |
| H | -1.204555 | -2.894864 | 0.088644 |
| H | 1.222362 | -2.548721 | 0.036423 |
| H | 4.369497 | -1.045251 | -0.532598 |
| H | 3.437926 | -1.951725 | 0.674467 |
| H | 3.006002 | -2.047097 | -1.046550 |
| H | 4.081453 | 1.158211 | -0.026504 |
| H | 2.493218 | 1.781630 | 0.475579 |
| H | 3.405689 | 0.682257 | 1.548042 |

Name: 7-Dimethylamino-4-nitroso-benzo[*c*]isoxazole anion (conformer B)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -662.5314087 a.u.

ZPE: 99.879 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | -1.514175 | 2.171479 | -0.062327 |
| C | -1.112301 | 0.812950 | -0.010729 |
| C | 0.326457 | 0.796327 | -0.057443 |
| N | 0.838533 | 2.011010 | -0.136696 |
| O | -0.365116 | 2.847929 | -0.131055 |
| C | -1.839635 | -0.410951 | 0.034485 |
| C | -1.131274 | -1.603881 | 0.040349 |
| C | 0.268529 | -1.620789 | 0.005334 |
| C | 1.041958 | -0.457508 | -0.051978 |
| N | -3.250260 | -0.368749 | 0.090461 |
| O | -3.830799 | -1.461148 | 0.077195 |
| N | 2.427921 | -0.510044 | -0.162965 |
| C | 3.255367 | 0.493921 | 0.497253 |
| C | 3.070290 | -1.801566 | -0.275407 |
| H | -1.683869 | -2.533090 | 0.092253 |
| H | 0.759295 | -2.584409 | 0.038397 |
| H | 4.115089 | -1.646942 | -0.551494 |
| H | 3.051007 | -2.379873 | 0.663769 |
| H | 2.597015 | -2.401131 | -1.054384 |
| H | 4.210990 | 0.572650 | -0.028603 |
| H | 2.751872 | 1.457535 | 0.474118 |
| H | 3.461267 | 0.215605 | 1.543989 |

Name: 5-Chloro-4-nitroso-benzo[*c*]isoxazole anion (conformer A)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -988.1444604 a.u.

ZPE: 48.046 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | -2.457105 | -0.203767 | 0.000000 |
| C | -1.035800 | -0.260946 | 0.000000 |
| C | -0.678893 | -1.661821 | 0.000000 |
| C | 0.686045 | -2.056810 | 0.000000 |
| C | 1.660335 | -1.093689 | 0.000000 |
| C | 1.321930 | 0.278162 | 0.000000 |
| C | 0.000000 | 0.715619 | 0.000000 |
| N | -1.721734 | -2.459107 | 0.000000 |
| N | -0.158264 | 2.135668 | 0.000000 |
| O | -2.827404 | -1.488926 | 0.000000 |
| O | -1.305253 | 2.550612 | 0.000000 |
| Cl | 2.681381 | 1.408593 | 0.000000 |
| H | 0.950931 | -3.108221 | 0.000000 |
| H | 2.707752 | -1.367764 | 0.000000 |

Name: 5-Chloro-4-nitroso-benzo[*c*]isoxazole anion (conformer B)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -988.1415040 a.u.

ZPE: 48.063 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | 0.350020 | 0.595210 | -0.042193 |
| C | -1.063443 | 0.502375 | -0.047485 |
| C | -1.716132 | -0.780100 | 0.028051 |
| C | -0.922640 | -1.959936 | 0.068870 |
| C | 0.443141 | -1.842200 | 0.048703 |
| C | 1.088241 | -0.581706 | 0.013041 |
| C | -2.082159 | 1.491020 | -0.070815 |
| N | -3.025230 | -0.684003 | 0.047378 |
| N | 0.899558 | 1.909683 | -0.217868 |
| O | -3.210142 | 0.786967 | -0.023127 |
| O | 1.974784 | 2.118596 | 0.318521 |
| Cl | 2.853126 | -0.629736 | -0.078462 |
| H | -1.388221 | -2.937866 | 0.112219 |
| H | 1.065478 | -2.728866 | 0.062888 |

Name: 5-Chloro-4-nitroso-benzo[*c*]isoxazole anion (transition state)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -988.0961482 a.u.

ZPE: 47.395 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | -1.038076 | -0.246000 | 0.000000 |
| C | 0.000000 | 0.782830 | 0.000000 |
| C | 1.345343 | 0.419447 | 0.000000 |
| C | 1.760634 | -0.912924 | 0.000000 |
| C | 0.799182 | -1.921320 | 0.000000 |
| C | -0.555729 | -1.618648 | 0.000000 |
| C | -2.370443 | 0.046910 | 0.000000 |
| N | -0.399843 | 2.081522 | 0.000000 |
| N | -1.485417 | -2.608296 | 0.000000 |
| O | -1.657472 | 2.168300 | 0.000000 |
| O | -2.652955 | -2.126687 | 0.000000 |
| Cl | 2.595579 | 1.656598 | 0.000000 |
| H | 1.093318 | -2.964778 | 0.000000 |
| H | 2.816614 | -1.144642 | 0.000000 |

Name: 7-Chloro-4-nitroso-benzo[*c*]isoxazole anion (conformer A)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -988.1518655 a.u.

ZPE: 48.393 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | -2.261344 | 0.452300 | 0.000000 |
| C | -0.994501 | -0.191534 | 0.000000 |
| C | 0.000000 | 0.867385 | 0.000000 |
| C | 1.377754 | 0.520302 | 0.000000 |
| C | 1.771619 | -0.792965 | 0.000000 |
| C | 0.808173 | -1.820897 | 0.000000 |
| C | -0.551415 | -1.537912 | 0.000000 |
| N | -1.331563 | -2.733856 | 0.000000 |
| N | -0.524360 | 2.067987 | 0.000000 |
| O | -1.965691 | 1.751650 | 0.000000 |
| O | -2.545928 | -2.602125 | 0.000000 |
| Cl | 2.602548 | 1.787048 | 0.000000 |
| H | 1.112303 | -2.860009 | 0.000000 |
| H | 2.827080 | -1.035008 | 0.000000 |

Name: 7-Chloro-4-nitroso-benzo[*c*]isoxazole anion (conformer B)

Level: B3-LYP/6-311+G(2d,p)

Total energy: -988.1518461 a.u.

ZPE: 48.204 kcal/mol

**Cartesian Coordinates**

| | | | |
|---|---|---|---|
| C | -0.805964 | -1.369263 | 0.000000 |
| C | -1.088848 | 0.015563 | 0.000000 |
| C | 0.000000 | 0.973024 | 0.000000 |
| C | 1.325905 | 0.470873 | 0.000000 |
| C | 1.567240 | -0.884217 | 0.000000 |
| C | 0.510779 | -1.811019 | 0.000000 |
| N | -0.410629 | 2.218861 | 0.000000 |
| O | -1.881700 | 2.033495 | 0.000000 |
| C | -2.294377 | 0.771951 | 0.000000 |
| N | -1.913881 | -2.275713 | 0.000000 |
| O | -1.624846 | -3.467315 | 0.000000 |
| Cl | 2.690093 | 1.586786 | 0.000000 |
| H | 0.711421 | -2.873628 | 0.000000 |
| H | 2.592522 | -1.234686 | 0.000000 |