**Table I.**  The structures and energies of RDX decomposition species on the adiabatic singlet ground state potential energy surface. Energies were determined at the B3LYP/cc-pVTZ//CCSD(T)/cc-pVTZ level of theory with B3LYP/cc-pVTZ zero point energy corrections.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | B3LYP/ cc-pVTZ + Ezpc a | Ezpc b | CCSD(T)/ cc-pVTZ | Ec (kJ/mol) |
|  | **RDX (C1, 1A)** | -897.604826 | 0.142310 | -896.129323 | 0 |
|  | **HNO (Cs, 1A')** | -130.509649 | 0.013837 | -130.298111 |  |
|  | **HONO (Cs, 1A')** | -205.765775 | 0.020217 | -205.433369 |  |
|  | i1 (C1, 1A) | -691.862429 | 0.115834 | -690.705910 |  |
|  | i2 (Cs, 1A') | -486.116226 | 0.090025 | -485.285807 |  |
|  | i3 (D3h, 1A1') | -280.396643 | 0.065169 | -279.894957 |  |
|  | tsi1 (C1, 1A) | -897.546291 | 0.134366 | -896.055557 |  |
|  | tsi1i2 (C1, 1A) | -691.801322 | 0.108128 | -690.631427 |  |
|  | tsi2i3 (C1, 1A) | -486.064968 | 0.082802 | -485.220819 |  |
|  | tsi2i12 (C1, 1A) | -486.013563 | 0.080557 | -485.168303 |  |
|  |  |  |  |  |  |
|  | **i1 + HONO** | -897.628204 | 0.136051 | -896.139279 | -43 |
|  | **i2 + 2HONO** | -897.647776 | 0.130459 | -896.152544 | -92 |
|  | **i3 + 3HONO** | -897.693968 | 0.125820 | -896.195062 | -216 |
|  | **tsi1** | -897.546291 | 0.134366 | -896.055557 | 173 |
|  | **tsi1i2 + HONO** | -897.567097 | 0.128345 | -896.064796 | 133 |
|  | **tsi2i3 + 2HONO** | -897.596518 | 0.123236 | -896.087556 | 60 |
|  | **tsi2i12 + 2HONO** | -897.545113 | 0.120991 | -896.035041 | 192 |
|  |  |  |  |  |  |
|  | i4 (Cs, 1A') | -897.573503 | 0.138745 | -896.095517 |  |
|  | i5 (C1, 1A) | -767.038907 | 0.119747 | -765.760826 |  |
|  | i6 (C1, 1A) | -767.028510 | 0.120146 | -765.762769 |  |
|  | i7 (C1, 1A) | -767.133860 | 0.121174 | -765.863440 |  |
|  | i8 (C1, 1A) | -561.396198 | 0.095001 | -560.448208 |  |
|  | i9 (Cs, 1A') | -355.664792 | 0.070080 | -355.042321 |  |
|  | i10 (Cs, 1A') | -355.664758 | 0.070318 | -355.045852 |  |
|  | i11 (C1, 1A) | -767.116315 | 0.120669 | -765.846140 |  |
|  | i12 (C1, 1A) | -486.151629 | 0.088926 | -485.325457 |  |
|  | 3i12 (C1, 3A) | -486.074384 | 0.087483 | -485.235178 |  |
|  | i13 (C2v, 2B1) | -280.929479 | 0.073224 | -280.427524 |  |
|  | i14 (C1, 2A) | -280.949763 | 0.073282 | -280.446031 |  |
|  | i15 (C1, 2A) | -692.404209 | 0.125581 | -691.254278 |  |
|  |  |  |  |  |  |
|  | tsi4 (C1, 1A) | -897.507337 | 0.134844 | -896.060958 |  |
|  | tsi4i5 (C1, 1A) | -897.522829 | 0.133008 | -896.040468 |  |
|  | tsi5i6 (C1, 1A) | -766.981604 | 0.118089 | -765.703292 |  |
|  | tsi6i7 (C1, 1A) | -766.956018 | 0.112575 | -765.713804 |  |
|  | tsi7i8 (C1, 1A) | -767.075930 | 0.113113 | -765.790344 |  |
|  | tsi7i11 (C1, 1A) | -767.063943 | 0.115508 | -765.785399 |  |
|  | tsi8i9 (C1, 1A) | -561.320614 | 0.090715 | -560.360181 |  |
|  | tsi9i10 (C1, 1A) | -355.608895 | 0.065136 | -354.982209 |  |
|  | tsi9i12 (C1, 1A) | -486.109471 | 0.083264 | -485.269482 |  |
|  | 3tsi12i14 | -486.069637 | 0.085827 | -485.218004 |  |
|  | tsi13i14 | -280.861812 | 0.068250 | -280.355942 |  |
|  |  |  |  |  |  |
|  | **i4** | -897.573503 | 0.138745 | -896.095517 | 79 |
|  | **i5 + HNO** | -897.548556 | 0.133584 | -896.058937 | 162 |
|  | **i6 + HNO** | -897.538159 | 0.133983 | -896.060880 | 158 |
|  | **i7 + HNO** | -897.643509 | 0.135011 | -896.161551 | -104 |
|  | **i8 + HNO + HONO** | -897.671622 | 0.129055 | -896.179687 | -167 |
|  | **i9 + HNO + 2HONO** | -897.705991 | 0.124351 | -896.207169 | -252 |
|  | **i10 + HNO + 2HONO** | -897.705957 | 0.124589 | -896.210699 | -260 |
|  | **i11 + HNO** | -897.625964 | 0.134506 | -896.144250 | -60 |
|  | **i12 + 2HONO** | -897.683179 | 0.129360 | -896.192194 | -199 |
|  | **3i12 + 2\*HONO** | -897.605934 | 0.127917 | -896.101915 | 34 |
|  | **i13 + NO2 + 2\*HONO** | -897.608200 | 0.122441 | -896.094360 | 40 |
|  | **i14 + NO2 + 2\*HONO** | -897.628484 | 0.122499 | -896.112868 | -9 |
|  | **i15 + NO2** | -897.551380 | 0.134364 | -896.054377 | 176 |
|  | **tsi4** | -897.507337 | 0.134844 | -896.060958 | 160 |
|  | **tsi4i5** | -897.522829 | 0.133008 | -896.040468 | 209 |
|  | **tsi5i6 + HNO** | -897.491253 | 0.131926 | -896.001403 | 309 |
|  | **tsi6i7 + HNO** | -897.465667 | 0.126412 | -896.011915 | 267 |
|  | **tsi7i8 + HNO** | -897.585579 | 0.126950 | -896.088455 | 67 |
|  | **tsi7i11 + HNO** | -897.573592 | 0.129345 | -896.083510 | 86 |
|  | **tsi8i9 + HNO + HONO** | -897.596038 | 0.124769 | -896.091660 | 53 |
|  | **tsi9i10 + HNO + 2HONO** | -897.650094 | 0.119407 | -896.147057 | -107 |
|  | **tsi9i12 + 2HONO** | -897.641021 | 0.123698 | -896.136219 | -67 |
|  | **3tsi12i14 + 2\*HONO** | -897.601187 | 0.126261 | -896.084741 | 75 |
|  | **tsi13i14 + NO2 + 2\*HONO** | -897.540533 | 0.117467 | -896.022778 | 215 |

a B3LYP/cc-pVTZ energy with zero-point energy correction in hartree.

b zero-point energy by B3LYP/cc-pVTZ in hartree.

c relative energy by CCSD(T)/cc-pVTZ with B3LYP/cc-pVTZ zero-point energy correction.