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PAPER

Liquid-phase decomposition mechanism for bis(triaminoguanidinium) azotetrazolate (TAGzT)

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Supplementary material

TAGzT decomposition reactions:

Table S1. Important reactions in the decomposition of TAGzT along with thermodynamics parameters (SI units) calculated at CBS-QB3 level of theory.

No.	Reaction	$\Delta G^{\ddagger}_{f}$[a] (kJ/mol)	$\Delta G^{\ddagger}_{r}$[b] (kJ/mol)	ΔH_{rxn}[c] (kJ/mol)
R1	$AzT^{2-} = INT4 + N_2$	156.9	122.6	84.5
R2	$INT4 + TAG^{+} = INT4a + TAG$	-13.4	63.2	-77.4
R3	$INT4a = INT4a1 + N_2$	103.3	251.5	-104.2
R4	$INT4 = INT4b + N_2$	10.0	247.3	-195.4
R5	$INT4b = 2CN^{-} + 2N_2$	135.6	632.2	-362.3
R6	$TAG = INT5 + NH_3$	182.8	247.3	-15.1
R7	$INT5 = INT5b + N_2$	113.0	184.1	-28.0
R8	$INT4a1 + TAG^{+} = TAG^{+} + CN^{-} + HCN + 2N_2$	156.9	696.6	-406.3
R9	$TAG^{+} + CN^{-} = TAG + HCN$	13.8	11.7	2.5
R10	$HNC + CN^{-} = HCN + CN^{-}$	0	65.0	-61.3
R11	$TAG^{+} + TAG = INT1$	130.5	56.9	13.0
R12	$INT1 = INT1a$	24.7	5.0	16.7
R13	$INT1a = INT1a1 + N_2H_4$	51.0	74.9	36.0
R14	$INT5 = N_2H_4 + HNC + N_2$	128.4	355.6	-138.1
R15	$INT1a1 = INT1a1b + NH_3$	154.0	196.2	7.1
R16	$INT1a1b + CN^{-} = TAG + HNNCN + HCN$	22.2	61.5	5.0
R17	$HNNCN + CN^{-} = N_2 + HCN + CN^{-}$	18.8	332.6	-289.1
R18	$HNNCN + NH_3 = N_2 + HCN + NH_3$	51.9	365.7	-289.1
R19	$INT1a1b = TAGiso2^{+} + HNNCN$	143.1	80.8	118.0
R20	$TAGiso2^{+} = TAG^{+}$	102.5	215.5	-112.5
R21	$INT4a1 = INT4a1b$	58.6	193.7	-143.9
R22	INT4a1b = 3-azido-1,2,4-triazol-4-ide	87.0	109.6	-14.6
R23	3-azido-1,2,4-triazol-4-ide = $INT4a1b2 + N_2$	131.0	193.7	-17.6
R24	$INT4a1b2 = INT4a1b3 + N_2$	39.7	172.0	-82.0
R25	$INT4a1b3 = HCN + CN^{-}$	105.0	283.7	-151.9
R26	3-azido-1,2,4-triazol-4-ide + HCN = 3-azido-1H-1,2,4-triazole + CN^{-}	22.2	23.4	-1.3
R27	3-azido-1H-1,2,4-triazole = $INT4a1b6 + N_2$	143.9	132.2	58.6

[a]Gibbs free energy of activation in the forward direction.
[b]Gibbs free energy of activation in the reverse direction.
[c]Enthalpy of reaction.

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XYZ coordinates for the transition states structures:

1. TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	16.113596	-6.663704	0.002036
2	7	0	15.580847	-7.868790	-0.104866
3	7	0	14.239267	-7.775693	-0.107851
4	6	0	13.995686	-6.455427	0.002803
5	7	0	15.137686	-5.744777	0.072667
6	7	0	12.773056	-5.788614	0.043526
7	7	0	11.751101	-6.583395	-0.012011
8	6	0	10.537101	-6.110929	0.007743
9	7	0	9.383250	-6.773897	-0.039989
10	7	0	8.250061	-6.409235	-0.032159
11	7	0	8.809216	-4.314829	0.080071
12	7	0	9.959832	-4.378809	0.088031

2. TS4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.777300	13.254601	0.590565
2	7	0	-5.089401	11.980044	0.774533
3	7	0	-6.325229	11.882795	1.286742
4	6	0	-6.737737	13.158655	1.401314
5	7	0	-5.800622	14.026100	0.977876
6	7	0	-7.952816	13.649948	1.877410
7	7	0	-8.787481	12.755627	2.266586
8	6	0	-9.970122	13.266966	2.726260
9	7	0	-10.831297	12.374699	3.135258
10	7	0	-11.697008	11.744991	3.533356
11	6	0	-10.462883	16.686003	3.903973
12	7	0	-9.894795	17.913141	4.009453
13	7	0	-11.288759	16.303966	4.901236
14	7	0	-10.226235	15.917921	2.856449
15	7	0	-9.222405	16.430042	1.964386
16	7	0	-10.065315	18.655319	5.189742
17	7	0	-12.076988	15.152015	4.772685
18	1	0	-9.128532	18.075874	3.363329
19	1	0	-11.470817	17.004437	5.610853
20	1	0	-10.264621	14.675702	2.872582
21	1	0	-13.058350	15.414435	4.753041
22	1	0	-11.921489	14.554630	5.577868
23	1	0	-9.195592	18.679909	5.715560
24	1	0	-10.321255	19.606311	4.946236
25	1	0	-8.579271	15.640127	1.814007
26	1	0	-9.679917	16.602634	1.071585

3. TS4a1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	7.888711	-6.023370	0.075426
2	7	0	7.276186	-7.199587	0.090512
3	7	0	5.953950	-7.024316	-0.034167
4	6	0	5.806329	-5.692044	-0.126823
5	7	0	6.982776	-5.047464	-0.062870
6	7	0	4.625608	-4.955731	-0.252397
7	7	0	3.574445	-5.672524	-0.363457
8	6	0	2.346803	-5.389381	-0.477875
9	7	0	1.447027	-6.818666	-0.590312
10	7	0	0.978448	-7.614004	-1.209826
11	1	0	1.706057	-4.791218	0.158327

4. TS4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.871155	-0.316497	0.008589
2	7	0	0.047192	0.461822	0.019830
3	6	0	-0.321633	1.926939	0.119989
4	7	0	-1.570855	2.196484	0.043834
5	7	0	-2.548766	1.326076	-0.104167
6	6	0	-3.816798	1.885818	-0.166101
7	7	0	-4.893272	1.082450	-0.313088
8	7	0	-5.947543	1.922716	-0.337231
9	7	0	-5.528755	3.163657	-0.212016
10	7	0	-4.181981	3.185148	-0.100991

5. TS4b1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.114568	-0.658638	0.062269
2	7	0	0.131758	0.719908	0.253304
3	7	0	1.220038	1.047429	0.869770
4	6	0	1.933766	-0.123217	1.105244
5	7	0	1.193918	-1.167687	0.560158
6	7	0	3.048086	-0.235567	1.812186
7	7	0	4.594950	-0.048099	0.484347
8	6	0	5.722153	-0.001441	0.160982

6. TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.854186	-9.922040	1.722985
2	7	0	10.509964	-9.828076	2.198013
3	7	0	12.473667	-8.781994	1.370337
4	7	0	12.331307	-11.140707	1.372183
5	7	0	9.589049	-9.846501	1.075087
6	7	0	13.585456	-8.834204	0.729982
7	7	0	11.674745	-11.551671	-0.196728
8	1	0	11.809780	-11.854828	1.875467
9	1	0	8.671638	-10.086728	1.435293
10	1	0	9.519945	-8.914541	0.668233
11	1	0	12.252805	-11.056440	-0.867609
12	1	0	13.885651	-7.864141	0.622058
13	1	0	11.717884	-12.554968	-0.355528
14	1	0	10.715211	-11.191157	-0.184965
15	1	0	10.407524	-8.954574	2.707223

7. TS5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.672266	2.738060	0.186450
2	7	0	-5.935095	3.215116	-0.144889
3	7	0	-3.721204	3.553067	0.396288
4	7	0	-4.409887	0.879771	-0.283121
5	7	0	-6.946678	2.227462	0.091203
6	1	0	-7.243124	2.177721	1.067710
7	1	0	-7.760363	2.411347	-0.492683
8	1	0	-6.205442	4.154274	0.155361
9	1	0	-2.853628	3.027446	0.529976
10	7	0	-5.396474	0.306976	-0.547839
11	1	0	-6.440907	1.201532	-0.251944

8. TS4a1j

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.381208	-2.106007	0.963829
2	6	0	1.528728	-1.906515	0.276558
3	7	0	2.294098	-0.777052	0.279603
4	7	0	3.343326	-1.066622	-0.428918
5	7	0	3.231495	-2.356684	-0.899285
6	7	0	2.120575	-2.877125	-0.472093
7	7	0	0.226862	1.669612	2.443400
8	6	0	0.198313	0.714609	3.416216
9	7	0	-0.105764	-0.530064	3.152874
10	7	0	0.533093	1.139322	4.679261

11	1	0	0.181916	-1.355508	1.710852
12	1	0	0.213824	0.495278	5.397248
13	1	0	0.748785	2.502240	2.692180
14	7	0	-0.979868	-1.763489	-0.014616
15	6	0	-1.841847	-2.065935	-0.706286
16	1	0	-2.654780	-2.323652	-1.354546
17	7	0	-0.172783	-1.330925	4.362776
18	1	0	-0.934945	-1.986441	4.217993
19	1	0	0.670655	-1.901941	4.401507
20	7	0	0.582519	2.525745	4.936996
21	1	0	-0.277384	2.837435	5.382853
22	1	0	1.351815	2.702870	5.573196
23	7	0	0.120011	1.278773	1.094708
24	1	0	-0.287859	2.049738	0.579352
25	1	0	1.038858	1.055126	0.713615

9. TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.651039	-1.515291	1.663972
2	6	0	-2.493538	-1.013944	0.629584
3	7	0	-2.345296	0.078761	-1.782468
4	6	0	-1.385797	0.413929	-2.619035
5	7	0	-0.087337	0.448796	-2.246288
6	7	0	-1.647744	0.697944	-3.924954
7	1	0	0.548864	0.848645	-2.926502
8	1	0	-2.301921	-0.442301	-0.567635
9	1	0	-2.634142	0.807266	-4.134222
10	7	0	-3.653694	0.098984	-2.374296
11	1	0	-4.011898	-0.853958	-2.373535
12	1	0	-4.254736	0.630561	-1.750236
13	7	0	-0.650539	1.308604	-4.707250
14	1	0	-0.580805	0.817478	-5.592153
15	1	0	-0.898267	2.276456	-4.895196
16	7	0	0.269401	0.285325	-0.901063
17	1	0	0.996304	-0.419744	-0.838585
18	1	0	0.639175	1.159055	-0.537176

10. No TS found for R10.

11. TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.208934	0.693127	0.209882
2	7	0	-1.738658	1.486949	-0.759785
3	7	0	-0.487403	1.356365	1.191113
4	7	0	-1.894248	-0.414700	0.761075
5	7	0	-3.039749	1.244158	-1.244160

6	7	0	0.078800	2.597368	0.817967
7	7	0	-2.491710	-1.321755	-0.160417
8	6	0	1.189166	-0.857374	-0.196951
9	7	0	0.172862	-0.318154	-0.833661
10	7	0	0.915203	-1.491030	0.984781
11	7	0	2.460983	-0.805484	-0.670151
12	7	0	0.430777	0.062921	-2.175040
13	7	0	1.740632	-1.161706	2.142211
14	7	0	3.436350	-1.693033	-0.166430
15	1	0	-2.529745	-0.071692	1.480330
16	1	0	-3.665643	1.965333	-0.895496
17	1	0	-3.023453	1.302258	-2.257154
18	1	0	-0.008394	3.236824	1.600133
19	1	0	1.067162	2.485833	0.602985
20	1	0	-2.684685	-2.172073	0.356983
21	1	0	-3.359528	-0.925745	-0.511910
22	1	0	-0.074863	-1.395831	1.209862
23	1	0	2.510841	-0.499671	-1.637725
24	1	0	-0.317562	-0.325007	-2.744652
25	1	0	0.340413	1.074396	-2.245425
26	1	0	1.491259	-1.868560	2.832447
27	1	0	2.685339	-1.418181	1.847921
28	1	0	3.511935	-2.509815	-0.768932
29	1	0	4.328962	-1.210650	-0.174652
30	1	0	-1.357725	2.428860	-0.774089
31	1	0	0.093242	0.757858	1.771349

12. TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	13.401323	-9.163052	0.392054
2	7	0	12.556583	-8.563283	-0.605803
3	7	0	13.655586	-8.260544	1.508351
4	7	0	12.729839	-10.346260	1.023557
5	7	0	11.232112	-8.387465	-0.085411
6	7	0	14.165586	-7.013567	1.039002
7	7	0	12.285602	-11.284151	0.034151
8	6	0	15.537896	-10.385510	0.505594
9	7	0	14.650482	-9.622312	-0.269991
10	7	0	15.083053	-10.918250	1.598331
11	7	0	16.827015	-10.416872	0.047908
12	7	0	14.650062	-9.991448	-1.644734
13	7	0	15.935392	-11.401131	2.613010
14	7	0	17.588833	-11.583016	0.313518
15	1	0	11.978240	-9.998351	1.621861
16	1	0	11.166349	-7.528150	0.457500
17	1	0	10.611024	-8.301999	-0.882100
18	1	0	13.858502	-6.292633	1.681517
19	1	0	15.182512	-7.015270	1.021816
20	1	0	12.113816	-12.162107	0.516026
21	1	0	11.398438	-10.944148	-0.330703
22	1	0	13.743960	-10.799194	1.569332
23	1	0	16.914443	-10.022756	-0.883219

24	1	0	13.865340	-10.620638	-1.805711
25	1	0	14.501670	-9.155650	-2.197724
26	1	0	15.385348	-12.052538	3.162739
27	1	0	16.707432	-11.905183	2.173268
28	1	0	17.502489	-12.239440	-0.459516
29	1	0	18.561943	-11.308384	0.392547
30	1	0	12.987706	-7.667206	-0.835154
31	1	0	14.262977	-8.689245	2.201969

13. TS1a1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.573036	0.797532	-0.209226
2	7	0	-1.388913	1.385064	-1.198347
3	7	0	-0.264451	1.492444	0.923237
4	7	0	-1.844199	-0.565474	0.447244
5	7	0	-2.684945	1.788657	-0.764269
6	7	0	-0.910470	2.711048	1.206672
7	7	0	-2.423375	-1.399649	-0.561789
8	6	0	1.456381	-0.567454	0.060595
9	7	0	0.453079	0.016782	-0.763895
10	7	0	1.144032	-0.881974	1.262915
11	7	0	2.690706	-0.653347	-0.568872
12	7	0	0.213251	-0.734387	-1.952832
13	7	0	2.159030	-1.236895	2.158610
14	7	0	3.452855	-1.824141	-0.292861
15	1	0	-2.534713	-0.066474	1.006882
16	1	0	-2.624149	2.683164	-0.282474
17	1	0	-3.252420	1.887646	-1.599085
18	1	0	-1.426968	2.627155	2.077935
19	1	0	-0.200061	3.426345	1.328872
20	1	0	-3.075597	-2.051189	-0.127359
21	1	0	-2.969811	-0.778996	-1.153559
22	1	0	-1.225244	-1.116097	1.041433
23	1	0	2.623253	-0.418056	-1.553399
24	1	0	-0.605636	-1.323958	-1.795276
25	1	0	-0.009250	-0.083592	-2.697273
26	1	0	1.728964	-1.765567	2.907325
27	1	0	2.877675	-1.794326	1.694886
28	1	0	3.207093	-2.566039	-0.945840
29	1	0	4.431677	-1.594954	-0.425723
30	1	0	-0.864112	2.112782	-1.680705
31	1	0	0.265145	1.009151	1.639366

14. TS5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.771526	-9.917015	1.391055
2	7	0	10.653996	-9.069731	1.804638

3	7	0	13.174600	-9.275004	2.319963
4	7	0	11.695333	-11.014380	0.778450
5	7	0	9.632042	-9.725856	2.569299
6	7	0	12.804347	-8.421488	3.031341
7	1	0	10.741177	-11.295064	0.530450
8	1	0	9.022086	-8.992629	2.923238
9	1	0	9.086350	-10.282207	1.914707
10	1	0	11.193864	-8.410512	2.479644
11	1	0	10.296866	-8.538580	1.005462

15. TS1a1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.347467	1.002169	-0.223949
2	7	0	-1.233889	1.384170	-1.154695
3	7	0	-0.380612	1.486889	1.018820
4	7	0	-2.510583	1.856896	-0.798072
5	7	0	-0.893490	2.770361	1.294989
6	6	0	1.719174	-0.189438	0.342369
7	7	0	0.603820	0.090030	-0.531831
8	7	0	1.415550	-0.712576	1.545711
9	7	0	2.953161	-0.380025	-0.220722
10	7	0	0.415082	-0.862178	-1.575128
11	7	0	2.338596	-1.397480	2.131093
12	7	0	3.116253	-2.001152	-0.615916
13	1	0	-2.573716	2.844983	-1.022990
14	1	0	-3.195062	1.350239	-1.351486
15	1	0	-1.746880	2.671664	1.836794
16	1	0	-0.205735	3.255305	1.864066
17	1	0	3.007169	0.049535	-1.142280
18	1	0	-0.489198	-1.317404	-1.476537
19	1	0	0.474233	-0.417769	-2.485721
20	1	0	1.954722	-1.664765	3.040527
21	1	0	3.077202	-2.400045	0.329433
22	1	0	2.330271	-2.294195	-1.199063
23	1	0	4.018434	-2.171602	-1.053191
24	1	0	-1.006050	1.244002	-2.129388
25	1	0	0.080812	0.927272	1.733705

16. TS7c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.611363	0.254488	-0.483250
2	7	0	2.918742	-0.418711	-0.454506
3	7	0	1.361650	1.347029	-0.998843
4	7	0	3.817754	0.267015	0.036249
5	6	0	-0.673211	-0.704680	-0.205206
6	7	0	0.652558	-0.723295	0.067558
7	7	0	-1.118781	0.077048	-1.196076

8	7	0	-1.473614	-1.492361	0.522736
9	7	0	1.066782	-1.662878	1.029483
10	7	0	-2.444977	0.547297	-1.303835
11	7	0	-2.692212	-1.954521	-0.007702
12	1	0	4.697003	-0.255229	-0.073058
13	1	0	-0.974110	-2.076920	1.186499
14	1	0	1.765026	-2.273116	0.617764
15	1	0	1.482050	-1.169217	1.813628
16	1	0	-3.049910	-0.265483	-1.365742
17	1	0	-2.690417	1.026420	-0.438747
18	1	0	-2.581846	-2.935644	-0.246500
19	1	0	-3.395786	-1.883495	0.719174
20	1	0	0.104569	2.201971	0.139232
21	1	0	-0.408207	0.724764	-1.541827
22	6	0	-0.615285	2.508910	0.917711
23	7	0	-1.377990	2.802190	1.727528

17. TS7d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.810756	0.676301	-0.000002
2	7	0	-1.347053	-0.826150	-0.000010
3	7	0	-1.149681	1.792282	0.000001
4	7	0	-0.567457	-1.715315	0.000003
5	1	0	0.525320	-1.187076	0.000018
6	6	0	1.426874	-0.102795	-0.000005
7	7	0	2.456167	0.439774	-0.000003

18. TS7e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.970122	-0.182479	0.469075
2	7	0	-0.499091	1.209603	-0.122372
3	7	0	-1.761543	-0.876497	0.961540
4	7	0	0.616671	1.331034	-0.519053
5	1	0	1.256417	0.233604	-0.376954
6	7	0	1.725061	-0.943686	-0.145392
7	1	0	2.662294	-0.967891	-0.539738
8	1	0	1.180252	-1.685827	-0.576521
9	1	0	1.793877	-1.142458	0.849421

19. TS7f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.734852	0.628203	-0.301606
2	7	0	2.778694	-0.314203	-0.176175

3	7	0	1.463676	1.750733	-0.555714
4	7	0	3.657690	0.058642	0.607301
5	6	0	-0.918254	-0.283607	-0.179075
6	7	0	0.314244	-0.651173	-0.188396
7	7	0	-1.168135	1.140237	-0.374006
8	7	0	-1.983505	-1.054622	0.028884
9	7	0	0.504212	-2.031321	0.017721
10	7	0	-1.675167	1.853863	0.763522
11	7	0	-3.263081	-0.529116	-0.185185
12	1	0	4.394120	-0.659558	0.589829
13	1	0	-1.832319	-2.052856	0.126935
14	1	0	1.444603	-2.244249	-0.297704
15	1	0	0.476558	-2.217825	1.020111
16	1	0	-2.562851	1.423360	1.012600
17	1	0	-1.013968	1.695931	1.521303
18	1	0	-3.669205	-0.967009	-1.006608
19	1	0	-3.838586	-0.751286	0.620380
20	1	0	-0.238860	1.582739	-0.628359
21	1	0	-1.820856	1.274145	-1.151852

20. TS7g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.222203	-0.007538	0.089604
2	7	0	1.376366	-0.582108	-0.000721
3	7	0	-0.609300	-1.119407	0.471020
4	7	0	-0.183450	1.235994	-0.087280
5	7	0	2.539652	0.134654	-0.295837
6	7	0	-1.666582	-1.508053	-0.397324
7	7	0	-1.525230	1.563010	0.151005
8	1	0	0.476303	1.932458	-0.415518
9	1	0	2.829108	0.651387	0.532945
10	1	0	3.264863	-0.543458	-0.500861
11	1	0	-2.276466	-0.703331	-0.530870
12	1	0	-1.242210	-1.734881	-1.292727
13	1	0	-1.560441	2.273208	0.875091
14	1	0	-1.919700	1.952429	-0.699647
15	1	0	0.624323	-1.598543	0.374477
16	1	0	-0.956999	-1.040033	1.425741

21. TS4a1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.020494	-0.657842	0.463063
2	6	0	0.382897	0.043026	-0.679152
3	7	0	0.434396	1.370631	-0.816054
4	7	0	0.952036	1.550676	-2.047665
5	7	0	1.192167	0.386061	-2.619658
6	7	0	0.822291	-0.590155	-1.774607

7	7	0	0.170508	-1.900002	0.204426
8	6	0	0.764622	-2.553734	-0.652710
9	1	0	0.361449	-3.296769	-1.329926

22. TS4a1b1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.002077	-0.594377	0.548806
2	6	0	0.402920	-0.008501	-0.573875
3	7	0	0.516084	1.366597	-0.848769
4	7	0	0.949416	1.399958	-2.068391
5	7	0	1.217412	0.545425	-2.850020
6	7	0	0.737167	-0.873300	-1.543609
7	7	0	0.075567	-1.953117	0.286807
8	6	0	0.516084	-2.079649	-0.958487
9	1	0	0.679134	-3.028162	-1.448568

23. TS4a1b2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.203698	-0.554040	-0.412976
2	6	0	2.054328	0.766987	-0.149942
3	1	0	2.863873	1.467039	-0.306993
4	7	0	-2.201685	0.014830	-0.277373
5	7	0	-3.284624	0.156716	-0.431302
6	7	0	0.866447	1.099564	0.311823
7	6	0	0.235921	-0.114087	0.328872
8	7	0	-0.992047	-0.354209	0.833139
9	7	0	1.037059	-1.110852	-0.124537

24. TS4a1b3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.425316	-0.905640	0.000000
2	6	0	-1.058077	0.948695	0.000001
3	1	0	-1.753030	1.789258	0.000002
4	7	0	0.178425	1.162777	0.000001
5	6	0	1.115960	0.122715	0.000000
6	7	0	2.262288	-0.172534	-0.000001
7	7	0	-0.393767	-1.426728	-0.000001

25. TS4a1b4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.779482	-0.332458	-0.000002
2	1	0	-2.708855	0.257769	0.000005
3	7	0	-0.824787	0.442659	0.000010
4	6	0	0.871145	-0.258118	-0.000002
5	7	0	2.002519	0.042467	-0.000005

26. TS4a1b5

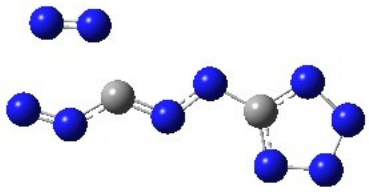
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.570113	-0.749812	-0.482678
2	6	0	-3.076752	0.468277	-0.328976
3	1	0	-3.705211	1.346302	-0.286365
4	7	0	0.730696	-0.568332	-0.189979
5	7	0	1.650856	0.067737	-0.082278
6	7	0	-1.745615	0.495528	-0.233807
7	6	0	-1.484246	-0.812022	-0.345192
8	7	0	-0.191105	-1.372140	-0.310693
9	7	0	-2.518173	-1.611802	-0.495121
10	1	0	-4.857465	-1.208199	-0.614120
11	6	0	-6.062657	-1.663618	-0.743247
12	7	0	-7.147282	-2.053874	-0.866371

27. TS4a1b6

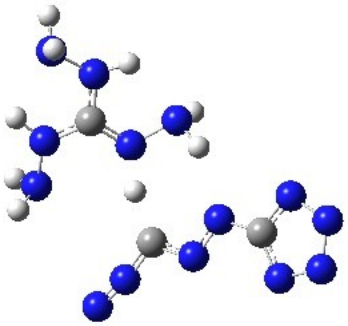
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.253847	0.000658	-0.285604
2	7	0	-0.991563	-0.484166	0.900109
3	7	0	0.785010	1.102237	0.417235
4	6	0	0.204674	-0.148929	0.377619
5	7	0	-3.309688	0.157469	-0.536470
6	7	0	1.025261	-1.084847	-0.130278
7	7	0	2.125676	-0.414362	-0.376762
8	6	0	1.978480	0.897289	-0.065638
9	1	0	2.769463	1.617074	-0.206958
10	1	0	2.950445	-0.873497	-0.746291

Transition states structures:

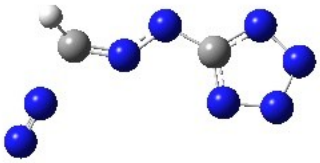
1. TS4



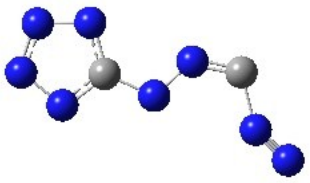
2. TS4a



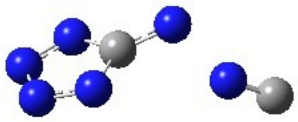
3. TS4a1



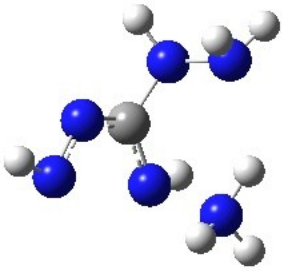
4. TS4b



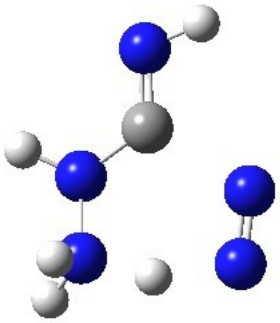
5. TS4b1



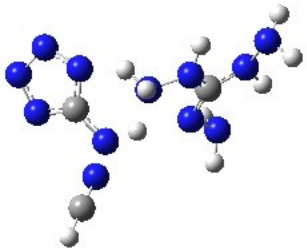
6. TS5



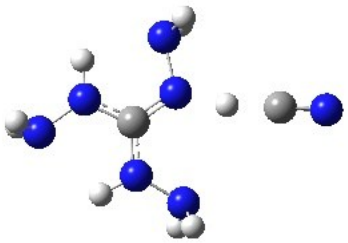
7. TS5b



8. TS4a1j

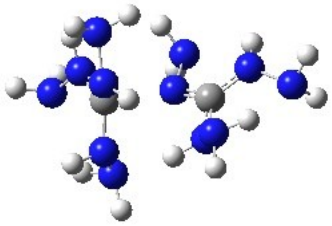


9. TS7

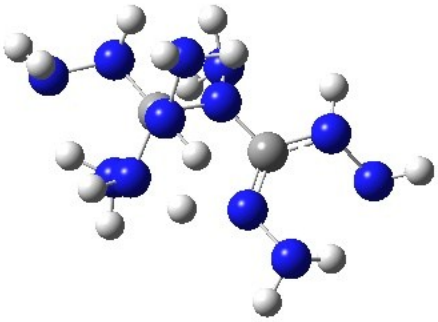


10. No TS found for R10.

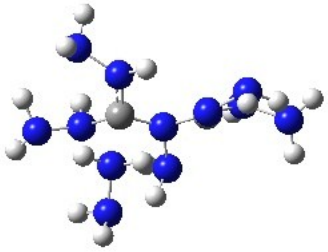
11. TS1



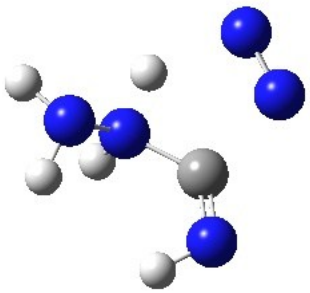
12. TS1a



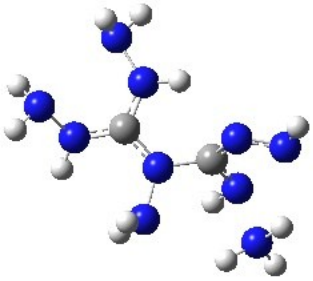
13. TS1a1



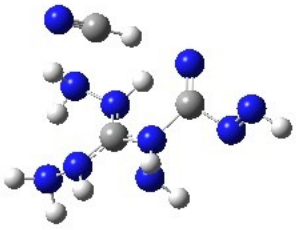
14. TS5a



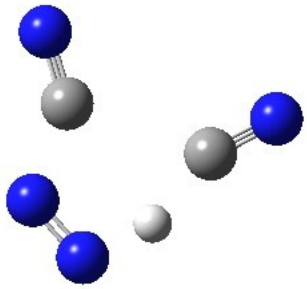
15. TS1a1b



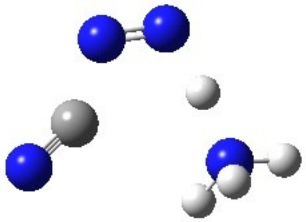
16. TS7c



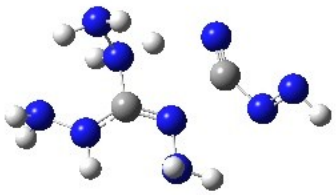
17. TS7d



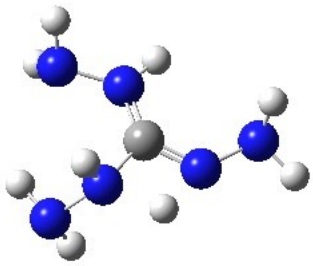
18. TS7e



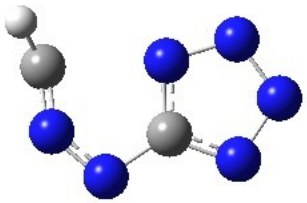
19. TS7f



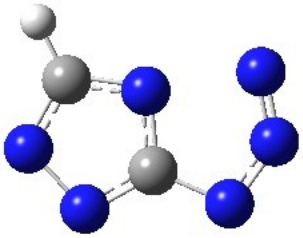
20. TS7g



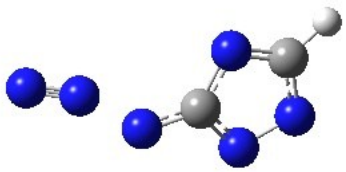
21. TS4a1b



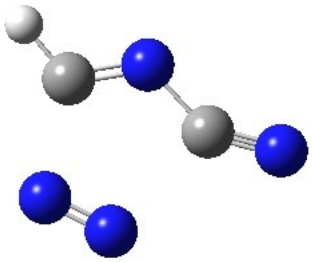
22. TS4a1b1



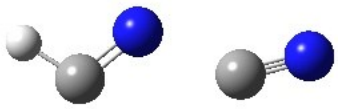
23. TS4a1b2



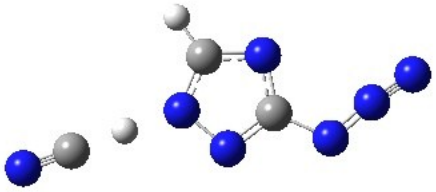
24. TS4a1b3



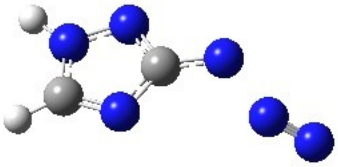
25. TS4a1b4



26. TS4a1b5



27. TS4a1b6



XYZ coordinates for the intermediate species structures:

1. AzT^{2-}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.856462	-0.336225	0.004823
2	7	0	3.367641	-1.576726	-0.079261
3	7	0	2.037321	-1.537833	-0.086040
4	6	0	1.741851	-0.226613	-0.003711
5	7	0	2.851359	0.532693	0.053501
6	7	0	0.493625	0.392414	0.027317
7	7	0	-0.494621	-0.392942	-0.028401
8	6	0	-1.742460	0.226709	0.003227
9	7	0	-2.852420	-0.531834	-0.053581
10	7	0	-3.857156	0.337331	-0.004457
11	7	0	-3.367383	1.577683	0.079728
12	7	0	-2.037183	1.537988	0.087065

2. TAG^{+}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.182632	2.980662	-0.054685
2	7	0	0.930718	3.701254	-0.209291
3	7	0	-1.364821	3.592593	0.048871
4	7	0	-0.113824	1.648141	-0.005129
5	7	0	1.138714	1.029162	-0.109625
6	7	0	0.834312	5.098237	-0.253598
7	7	0	-2.518059	2.816062	0.221483
8	1	0	1.805533	3.193304	-0.282255
9	1	0	-1.367246	4.606148	0.013047
10	1	0	-0.984306	1.142675	0.118572
11	1	0	-3.161796	2.996029	-0.542823
12	1	0	-2.967100	3.070476	1.095994
13	1	0	1.383903	5.497282	0.501332
14	1	0	1.201558	5.432352	-1.139381
15	1	0	1.316870	0.486669	0.730124
16	1	0	1.139303	0.404764	-0.910365

3. TAG

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.212538	2.855414	-0.124412
2	7	0	0.930449	3.629548	0.042066
3	7	0	-1.392973	3.570133	-0.161413
4	7	0	-0.175502	1.566352	-0.230063
5	7	0	1.197550	1.082596	-0.251560

6	7	0	0.818870	5.028620	-0.151802
7	7	0	-2.608596	2.899269	0.096579
8	1	0	1.744929	3.157026	-0.343503
9	1	0	-1.284562	4.521283	0.173003
10	1	0	-3.326012	3.335331	-0.472155
11	1	0	-2.871976	3.023165	1.072273
12	1	0	1.467604	5.485355	0.479168
13	1	0	1.072378	5.282813	-1.104349
14	1	0	1.506242	0.959634	0.714351
15	1	0	1.134605	0.141550	-0.625477

4. INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.021438	-0.633800	-0.008410
2	7	0	3.433968	-1.815073	-0.098930
3	7	0	2.098512	-1.661028	-0.103502
4	6	0	1.912730	-0.327944	-0.008256
5	7	0	3.089170	0.328928	0.050843
6	7	0	0.724980	0.401692	0.027558
7	7	0	-0.340934	-0.329839	-0.021922
8	6	0	-1.512439	0.373289	0.008536
9	7	0	-2.595268	-0.334489	-0.037466
10	7	0	-3.672640	-0.752532	-0.067563

5. INT4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.498003	-0.102874	0.533254
2	7	0	3.168921	-1.364322	0.258285
3	7	0	1.848633	-1.462571	0.096740
4	6	0	1.397857	-0.208757	0.286181
5	7	0	2.398066	0.648840	0.557245
6	7	0	0.090337	0.265952	0.235103
7	7	0	-0.789815	-0.610957	-0.035616
8	6	0	-2.058128	-0.103105	-0.076398
9	7	0	-3.027604	-0.944843	-0.353450
10	7	0	-3.878197	-1.653091	-0.590651
11	1	0	-2.335709	0.929485	0.097258

6. INT4a1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.944468	-0.997239	-0.080634
2	7	0	3.068743	-1.854051	0.413301

3	7	0	1.833642	-1.324239	0.357434
4	6	0	2.029459	-0.120567	-0.193526
5	7	0	3.313777	0.121287	-0.476554
6	7	0	1.044497	0.838175	-0.475941
7	7	0	-0.121886	0.524089	-0.199914
8	6	0	-1.283110	0.256872	-0.132040
9	1	0	-1.982431	0.386328	0.681761

7. INT4a1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.021213	-0.628183	0.612832
2	6	0	0.363980	0.074714	-0.456987
3	7	0	0.524701	1.348737	-0.885310
4	7	0	0.971983	1.232226	-2.145952
5	7	0	1.110187	-0.008330	-2.557559
6	7	0	0.722707	-0.755380	-1.481341
7	7	0	0.104146	-1.950743	0.235112
8	6	0	0.545944	-2.029679	-1.008671
9	1	0	0.737436	-2.931469	-1.564410

8. 3-azido-1,2,4-triazol-4-ide

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.323313	-0.266015	0.000005
2	6	0	-1.796668	0.946156	0.000011
3	1	0	-2.411423	1.836564	0.000020
4	7	0	2.021273	-0.080035	-0.000011
5	7	0	2.946863	0.560581	-0.000011
6	7	0	-0.454518	0.992654	0.000007
7	6	0	-0.205099	-0.315923	-0.000002
8	7	0	1.092417	-0.880904	-0.000010
9	7	0	-1.249720	-1.120182	-0.000004

9. INT4a1b2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.237228	0.801856	-0.000001
2	6	0	-1.256300	-0.636062	0.000000
3	1	0	-2.204269	-1.155872	0.000001
4	7	0	-0.097797	-1.169237	-0.000004
5	6	0	0.808891	-0.043500	-0.000003
6	7	0	2.064528	-0.040567	0.000002
7	7	0	-0.034230	1.152079	-0.000004

10. INT4a1b3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.564589	-0.420871	-0.000003
2	1	0	-2.528304	0.133372	0.000005
3	7	0	-0.620158	0.505260	0.000006
4	6	0	0.636444	0.071562	0.000000
5	7	0	1.770127	-0.195076	-0.000004

11. 3-azido-1H-1,2,4-triazole

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.007772	0.003206	0.046362
2	7	0	1.099085	0.831986	0.132206
3	7	0	-0.485743	-0.989610	-0.134172
4	6	0	-0.198797	0.314574	0.034099
5	7	0	2.917748	-0.648515	-0.015118
6	7	0	-1.208835	1.145367	0.112344
7	7	0	-2.238828	0.290621	-0.019383
8	6	0	-1.803636	-0.954583	-0.163920
9	1	0	-2.465944	-1.797062	-0.285502
10	1	0	-3.194679	0.619009	-0.005551

12. INT4a1b6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.612584	0.666411	1.141699
2	7	0	-0.948454	-1.058851	0.429754
3	6	0	-0.450884	0.272409	0.575830
4	7	0	-1.375631	1.163898	-0.043619
5	7	0	-2.289543	0.421092	-0.484220
6	6	0	-2.049049	-0.940412	-0.205449
7	1	0	-2.748799	-1.699006	-0.520784
8	1	0	-3.095089	0.800933	-0.982280

13. INT4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.574839	2.558817	0.132195
2	7	0	-1.586220	1.962885	0.008806
3	7	0	-2.628211	1.168098	-0.131257
4	6	0	-3.831648	1.848375	-0.182310
5	7	0	-4.996047	1.178425	-0.328420

6	7	0	-5.942652	2.146313	-0.335336
7	7	0	-5.381375	3.322709	-0.201606
8	7	0	-4.033728	3.179972	-0.100557

14. INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.837490	-9.852124	1.531814
2	7	0	10.586314	-9.373716	1.740413
3	7	0	12.807981	-8.811123	1.785714
4	7	0	12.213271	-11.041507	1.260169
5	7	0	9.495209	-10.206054	1.476566
6	7	0	13.678075	-8.725622	0.918546
7	1	0	11.382315	-11.627995	1.177885
8	1	0	8.847270	-10.150590	2.254450
9	1	0	9.017244	-9.890412	0.638051
10	1	0	14.321380	-7.977334	1.208883
11	1	0	10.451618	-8.371856	1.784370

15. INT5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.160925	-0.190312	0.566749
2	7	0	-0.472918	1.162942	0.895937
3	7	0	-0.494588	-0.989807	1.530017
4	7	0	-0.587138	1.976654	-0.269630
5	1	0	-0.422949	2.959883	-0.046414
6	1	0	-1.493511	1.887584	-0.740288
7	1	0	-0.212591	-1.932360	1.274453
8	1	0	0.134817	1.658503	-0.924803
9	1	0	-1.292201	1.315186	1.483845

16. INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.983642	0.596051	-0.033463
2	7	0	-1.718191	1.285423	-1.083234
3	7	0	-0.708851	1.497022	1.073962
4	7	0	-1.711618	-0.526509	0.538887
5	7	0	-3.072332	1.503803	-0.668324
6	7	0	-0.042899	2.679771	0.641750
7	7	0	-2.036870	-1.482279	-0.480380
8	6	0	1.219762	-0.610387	0.018727
9	7	0	0.277722	0.077811	-0.692812
10	7	0	0.908339	-1.125601	1.194749

11	7	0	2.462246	-0.690380	-0.512331
12	7	0	0.376691	-0.078159	-2.096760
13	7	0	1.843917	-1.396200	2.235952
14	7	0	3.295772	-1.774780	-0.154654
15	1	0	-2.550887	-0.138292	0.965817
16	1	0	-3.150172	2.359849	-0.122214
17	1	0	-3.625749	1.619186	-1.509543
18	1	0	-0.341052	3.443092	1.238017
19	1	0	0.966985	2.588931	0.724934
20	1	0	-2.202852	-2.368611	-0.016037
21	1	0	-2.902594	-1.202657	-0.938323
22	1	0	-0.092809	-1.132526	1.419921
23	1	0	2.500878	-0.352172	-1.469293
24	1	0	-0.403865	-0.663755	-2.388340
25	1	0	0.261021	0.829669	-2.532487
26	1	0	1.384634	-2.074661	2.838678
27	1	0	2.624039	-1.878795	1.783014
28	1	0	3.210689	-2.517914	-0.844844
29	1	0	4.254732	-1.443336	-0.155774
30	1	0	-1.236099	2.173684	-1.226641
31	1	0	-0.235322	1.034508	1.843455

17. INT1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.870632	0.629681	-0.099913
2	7	0	-1.685805	1.273397	-1.092981
3	7	0	-0.643006	1.464567	1.069078
4	7	0	-1.693172	-0.542818	0.469048
5	7	0	-2.985401	1.550483	-0.553444
6	7	0	-0.180802	2.757748	0.680422
7	7	0	-2.081930	-1.473624	-0.554788
8	6	0	1.272395	-0.561738	0.092200
9	7	0	0.351294	0.139613	-0.725780
10	7	0	0.854012	-1.047812	1.208593
11	7	0	2.567512	-0.540796	-0.397843
12	7	0	0.343513	-0.315458	-2.077212
13	7	0	1.787278	-1.468142	2.175075
14	7	0	3.341843	-1.715313	-0.179556
15	1	0	-2.484924	-0.125730	0.971186
16	1	0	-2.982735	2.425526	-0.032386
17	1	0	-3.617771	1.653535	-1.339140
18	1	0	-0.519261	3.423552	1.365562
19	1	0	0.835645	2.795719	0.676450
20	1	0	-2.431008	-2.303908	-0.082040
21	1	0	-2.860522	-1.045529	-1.050215
22	1	0	-0.999403	-1.008490	1.101501
23	1	0	2.591500	-0.189209	-1.349717
24	1	0	-0.409039	-0.991925	-2.189481
25	1	0	0.153517	0.476154	-2.680059
26	1	0	1.300236	-2.107703	2.791702
27	1	0	2.563114	-1.953541	1.722119
28	1	0	3.203744	-2.374129	-0.943536

29	1	0	4.318654	-1.443153	-0.168490
30	1	0	-1.197534	2.132540	-1.344331
31	1	0	-0.015530	1.001701	1.721160

18. INT1a1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.470590	0.972698	-0.247510
2	7	0	-1.288241	1.555187	-1.132550
3	7	0	-0.502585	1.287105	1.041365
4	7	0	-2.515818	2.117504	-0.732370
5	7	0	-0.932386	2.565141	1.469978
6	6	0	1.493246	-0.516893	0.076380
7	7	0	0.398450	0.005847	-0.697040
8	7	0	1.350135	-0.599083	1.345163
9	7	0	2.616628	-0.795271	-0.689631
10	7	0	0.198931	-0.620261	-1.943014
11	7	0	2.461000	-0.861649	2.147793
12	7	0	3.371322	-1.935956	-0.288915
13	1	0	-2.453881	3.129145	-0.793639
14	1	0	-3.225578	1.791126	-1.381582
15	1	0	-1.814464	2.456069	1.961998
16	1	0	-0.239742	2.898059	2.135152
17	1	0	2.417303	-0.762352	-1.683135
18	1	0	-0.704134	-1.082484	-1.975483
19	1	0	0.304591	0.025953	-2.716507
20	1	0	2.118185	-1.234767	3.024467
21	1	0	3.090109	-1.525867	1.694927
22	1	0	3.017372	-2.772051	-0.749730
23	1	0	4.329436	-1.789094	-0.586789
24	1	0	-1.062151	1.512336	-2.116020
25	1	0	0.030156	0.656951	1.651843

19. INT1a1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.973425	0.724798	-0.207878
2	7	0	-1.841696	1.096986	-1.149386
3	7	0	-1.081325	1.167138	1.039845
4	7	0	-3.134944	1.556293	-0.823144
5	7	0	-1.716880	2.403022	1.316671
6	6	0	1.166158	-0.602940	0.184495
7	7	0	0.038513	-0.150031	-0.587623
8	7	0	1.000408	-0.403107	1.607365
9	7	0	2.203896	-1.119132	-0.298942
10	7	0	0.085358	-0.615367	-1.906627
11	7	0	1.597627	-1.232276	2.305202
12	1	0	-3.173569	2.560654	-0.967860
13	1	0	-3.778830	1.106032	-1.467007

14	1	0	-2.571512	2.213798	1.831849
15	1	0	-1.088156	2.921291	1.924318
16	1	0	2.133599	-1.157106	-1.317507
17	1	0	-0.707546	-1.204117	-2.133768
18	1	0	0.243844	0.125354	-2.580355
19	1	0	1.424625	-0.966417	3.285809
20	1	0	-1.619319	0.912273	-2.116599
21	1	0	-0.438626	0.758633	1.720442

20. TAGiso2^{+}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.884054	-0.281887	-0.100056
2	7	0	0.347862	-0.594226	-0.077654
3	7	0	-1.157636	1.136483	-0.319566
4	7	0	-1.991767	-1.044911	0.131482
5	7	0	0.625660	-1.948396	0.109302
6	7	0	-1.571694	1.893373	0.831981
7	7	0	-3.216523	-0.530734	-0.343870
8	1	0	-1.850061	-2.046036	0.048768
9	1	0	1.623336	-2.036433	0.253566
10	1	0	0.157525	-2.329280	0.930524
11	1	0	-2.492410	1.542202	1.088732
12	1	0	-0.926456	1.650140	1.581098
13	1	0	-3.475176	-1.000758	-1.206399
14	1	0	-3.930116	-0.714110	0.351743
15	1	0	-0.306320	1.563271	-0.696204
16	1	0	-1.900200	1.233825	-1.021948

21. HNNCN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.186658	0.334941	1.314592
2	7	0	1.464507	1.378473	0.472254
3	7	0	0.884641	-0.432320	2.121030
4	7	0	2.066247	1.055199	-0.561798
5	1	0	2.210409	1.922098	-1.097281

22. N_2H_4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.216213	-0.851824	-2.318274
2	7	0	2.653839	-0.988340	-2.312599
3	1	0	3.042989	-0.778049	-3.230205
4	1	0	2.856475	-1.966488	-2.134819

5	1	0	1.014080	0.128680	-2.152861
6	1	0	0.833337	-1.071788	-3.236310

23. NH_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.686259	2.956323	0.077458
2	1	0	1.087215	2.021634	0.077493
3	1	0	1.087231	3.423622	0.886940
4	1	0	1.087176	3.423682	-0.732058

24. HCN

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.582760	1.407507	0.000000
2	1	0	-2.651623	1.407507	0.000000
3	7	0	-0.434326	1.407507	0.000000

25. HNC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	11.972067	-10.012906	1.397069
2	7	0	11.386291	-10.836895	0.822336
3	1	0	10.881875	-11.552169	0.323471

26. N_2

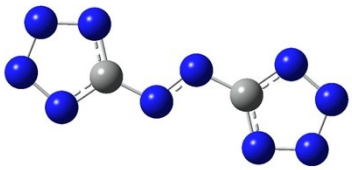
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.319537	1.956672	-0.086321
2	7	0	1.224360	1.956672	-0.086321

27. CN^-

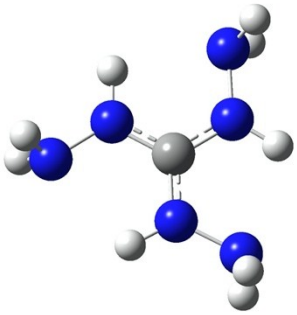
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.280314	-0.759847	1.220566
2	6	0	0.398443	-0.311217	0.378683

Intermediate species structures:

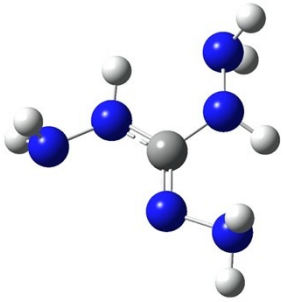
1. AzT^{2-}



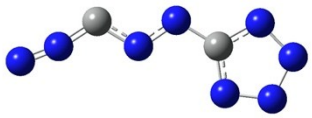
2. TAG^{+}



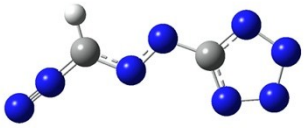
3. TAG



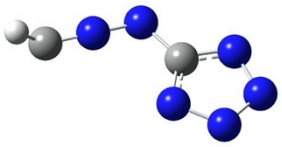
4. INT4



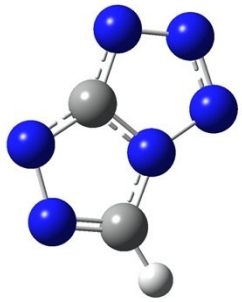
5. INT4a



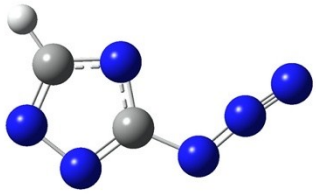
6. INT4a1



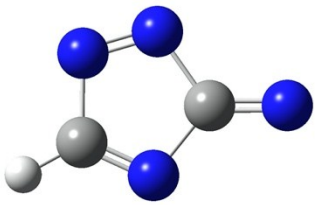
7. INT4a1b



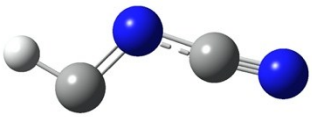
8. 3-azido-1,2,4-triazol-4-ide



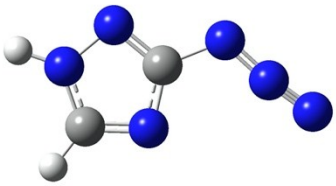
9. INT4a1b2



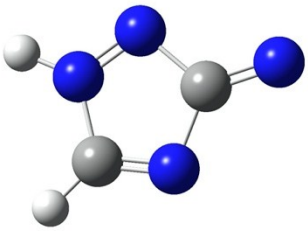
10. INT4a1b3



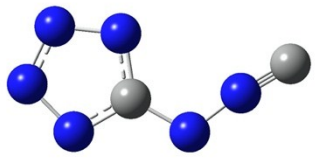
11. 3-azido-1H-1,2,4-triazole



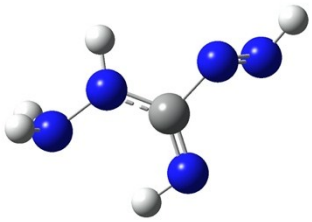
12. INT4a1b6



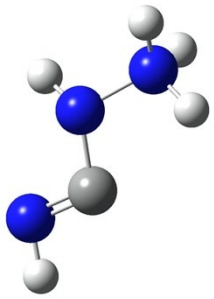
13. INT4b



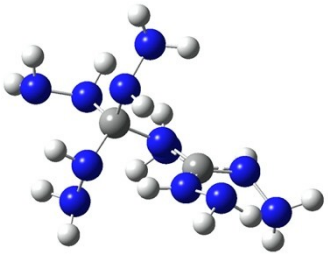
14. INT5



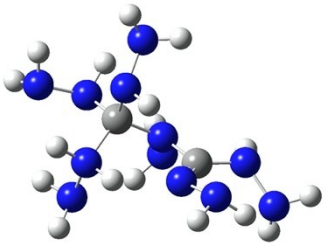
15. INT5b



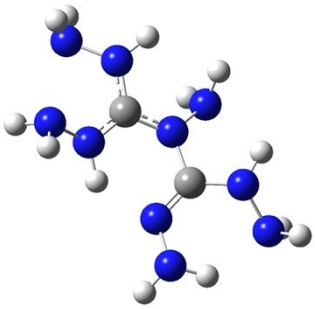
16. INT1



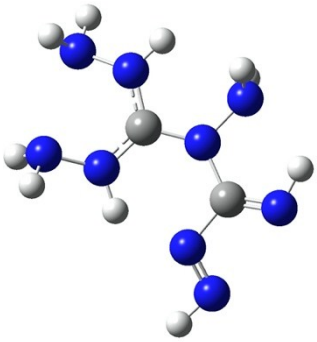
17. INT1a



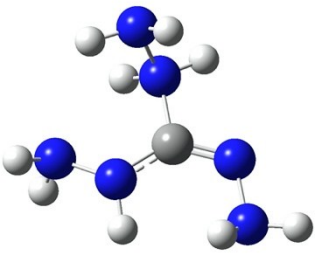
18. INT1a1



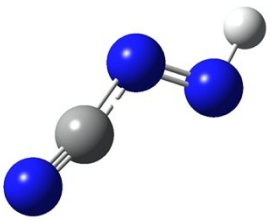
19. INT1a1b



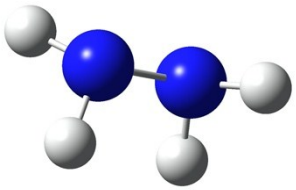
20. TAGiso2^{+}



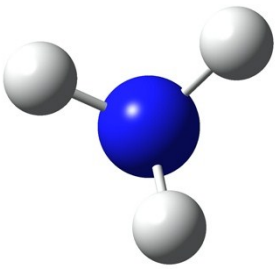
21. HNNCN



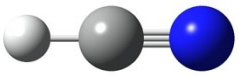
22. N_2H_4



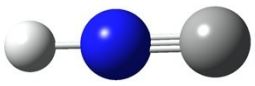
23. NH_3



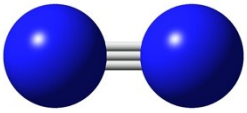
24. HCN



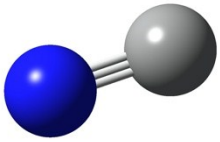
25. HNC



26. N_2



27. CN^-



Calculated frequencies of $N=N^{+}=N^{-}$ asymmetric stretch:

Table S2. Calculated frequencies of $N=N^{+}=N^{-}$ asymmetric stretch in 3-azido-1,2,4-triazol-4-ide anion and 3-azido-1H-1,2,4-triazole.

	3-azido-1,2,4-triazol-4-ide		**3-azido-1*H*-1,2,4-triazole**	
Level of Theory	Harmonic	Anharmonic	Harmonic	Anharmonic
B3LYP/6-311++G(d,p)	2218	2183	2251	2187
B3LYP/N07D	2226	2190	2258	2196
B3LYP/aug-cc-pVTZ	2215	2148	2249	2187
B2PLYP/6-311++G(d,p)	2173	2105	2190	2138
B2PLYP/N07D	2186	2134	2203	2153
B2PLYP/aug-cc-pVTZ	2164	*	2183	*
CBS-QB3(B3LYP/6-311G(2d,d,p))	2229	2189	2261	2200

* Calculation did not converge.

