Supporting Information

Theoretical screening of bistriazole-derived energetic salts with high energetic properties and low sensitivity

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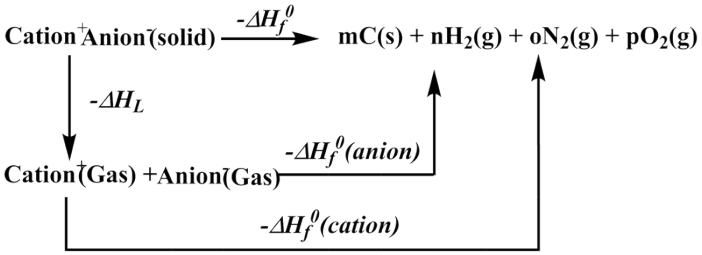

Scheme S1. Born−Haber energy cycle for the formation of the salts

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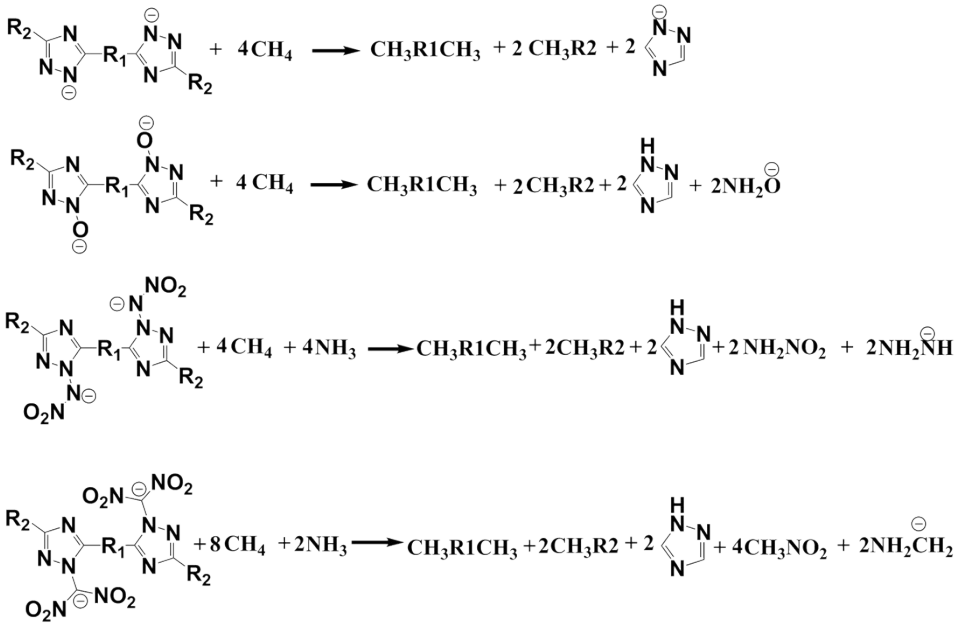
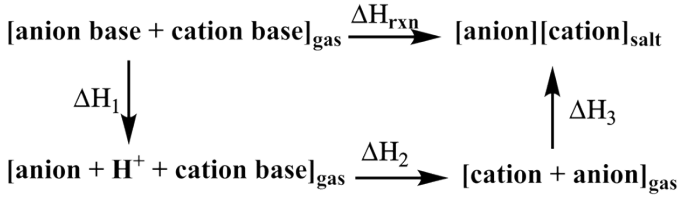


Scheme S2. Isodesmic reactions for the anions.



Scheme S3. Born−Haber cycle for the formation of the salts

Table S1. Volumes ($cm^3\ mol^{-1}$) and densities ($g\ cm^{-3}$) of the salts

Salts	V	A_s^+	V_s^+	A_s^-	V_s^-	ρ
A1	163.05	61.68	152.51	226.28	–155.43	1.71
A2	171.32	61.68	152.51	242.08	–149.09	1.73
A3	181.02	61.68	152.51	256.75	–142.99	1.73
A4	178.56	61.68	152.51	253.89	–144.84	1.74
A5	184.77	61.68	152.51	261.83	–143.45	1.77
A6	261.68	61.68	152.51	359.28	–128.75	1.92 (1.97) [a]
A7	269.1	61.68	152.51	374.25	–124.67	1.93
A8	281.83	61.68	152.51	390.81	–120.27	1.91
A9	276.56	61.68	152.51	386.7	–121.91	1.93
A10	285.51	61.68	152.51	391.61	–125.58	1.93
B1	176.44	61.68	152.51	242.56	–150.35	1.77 (1.9) [b]
B2	185.76	61.68	152.51	261.73	–144.35	1.78
B3	194.26	61.68	152.51	275.96	–138.11	1.78
B4	188.57	61.68	152.51	272.3	–140.87	1.82
B5	197.62	61.68	152.51	278.92	–139.28	1.82
B6	271.38	61.68	152.51	376	–125.69	1.98 (1.99) [c]
B7	282.51	61.68	152.51	394.76	–122.14	1.96

B8	293.52	61.68	152.51	417.69	–115.54	1.95
B9	289.18	61.68	152.51	404.98	–119.51	1.96
B10	291.16	61.68	152.51	405.19	–123.93	2.00
C1	213.38	61.68	152.51	315.31	–135.61	1.90 (1.86) [d]
C2	223.08	61.68	152.51	325.43	–131.88	1.90
C3	238.1	61.68	152.51	344.52	–127.2	1.86
C4	238.21	61.68	152.51	342.94	–128.36	1.85
C5	238.24	61.68	152.51	349.69	–126.17	1.91
C6	323.85	61.68	152.51	446.43	–119.36	1.96
C7	331.41	61.68	152.51	447.13	–117.51	1.97
C8	334.08	61.68	152.51	475	–112.62	2.00
C9	337.31	61.68	152.51	476.92	–112.18	1.97
C10	341.41	61.68	152.51	482.45	–111.35	2.00
D1	259.48	61.68	152.51	366.5	–127.63	1.94 (1.86) [e]
D2	271.2	61.68	152.51	385.15	–122.44	1.92
D3	281.28	61.68	152.51	401.41	–117.95	1.91
D4	277.28	61.68	152.51	401.87	–119.11	1.93
D5	281.85	61.68	152.51	399.77	–120.9	1.95
D6	355.11	61.68	152.51	499.74	–114.63	2.05
D7	371.82	61.68	152.51	511.85	–111.36	2.01
D8	380.91	61.68	152.51	531.56	–106.36	2.01
D9	381.98	61.68	152.51	535.38	–107.19	2.00
D10	375.36	61.68	152.51	534.93	–107.5	2.07

[a] The value is from Ref[1] ; [b] The value is from Ref[2]; [c] At the B3LYP/aug-cc-pVTZ level; [d] The value is from Ref[3]; [e] The value is from Ref[4].

Table S2. Calculated and experimental gas-phase heats of formation (kJ mol^{-1}) for small molecules and ions at 298 K

Molecules/ions	ΔH_f^o**(calculated)**	ΔH_f^o**(literature)**
CH_4	−73.6	−74.4[a]
NH_3	−45.3	−46.1[a]
CH_3NO_2	–85.9	–80.8[a]
$CH_3C(NO_2)_3$	–23.2	
NH_2NO_2	–3.9	–3.2[a]
CH_3CH_3	–84	–87[a]
CH_3NHCH_3	–18.8	–19.1[a]
$CH_3NHNHCH_3$	92.2	93.5[a]
$CH_3N{=}NCH_3$	151.5	153.2[a]
$CH_3N{=}N(O)CH_3$	–40.16	
1,2,4-triazole	192.9	192.9[a]
H^+		1536.2
NH_2O^-	37.21[b]	36.5[c]
NH_2NH^-	223.92[b]	225.2[c]
$NH_2CH_2^-$	196.11[b]	193.4[c]

1,2,4-triazolide	102.8[b]	

[a] The values were taken from Ref[5]. [b] The values were predicted by protonation reactions: $NH_2O^- + H^+ = NH_2OH$, $NH_2NH^- + H^+ = NH_2NH_2$, $NH_2CH_2^- + H^+ = NH_2CH_3$, 1,2,4-triazolide + H^+ = 1,2,4-triazole. [c] The values were taken from Ref[6].

Table S3. The HOFs ((kJ mol^{-1}) of cage anions, ammonium-based cation, and their salts and lattice energies of these salts

Salts	ΔH_f^o (cation)	ΔH_f^o (anion)	Lattice energy	ΔH_f^o (salt)
A1	678.80	258.95	1338.87	277.69
A2	678.80	261.65	1317.99	301.26
A3	678.80	344.77	1294.99	407.39
A4	678.80	431.29	1300.50	488.40
A5	678.80	301.91	1285.45	374.06
A6	678.80	279.11	1140.78	495.93
A7	678.80	282.31	1129.78	510.13
A8	678.80	366.48	1112.20	611.88
A9	678.80	464.94	1119.14	703.40
A10	678.80	376.16	1106.56	627.20
B1	678.80	110.71	1304.25	164.06 (213)[a]
B2	678.80	82.48	1282.98	157.10
B3	678.80	158.59	1264.41	251.78
B4	678.80	262.29	1276.13	343.76
B5	678.80	153.54	1256.37	254.77
B6	678.80	148.22	1125.68	380.13 (358.61) [b]
B7	678.80	126.47	1110.35	373.72
B8	678.80	210.63	1095.96	472.27
B9	678.80	312.36	1101.29	568.67
B10	678.80	237.38	1097.89	497.09
C1	678.80	288.21	1223.49	422.31 (535)[c]
C2	678.80	263.28	1205.47	415.41
C3	678.80	362.19	1179.92	539.87
C4	678.80	512.60	1179.85	690.35
C5	678.80	376.81	1178.78	555.63
C6	678.80	348.34	1058.01	647.93
C7	678.80	463.48	1049.23	771.85
C8	678.80	408.72	1045.97	720.35
C9	678.80	554.25	1042.70	869.15
C10	678.80	448.45	1037.82	768.22
D1	678.80	-30.40	1144.01	183.18 (360)[d]
D2	678.80	-51.50	1127.06	179.03
D3	678.80	35.25	1113.04	279.81
D4	678.80	175.93	1118.36	415.17
D5	678.80	98.03	1111.43	344.20
D6	678.80	40.85	1022.38	376.07

D7	678.80	39.46	1006.09	390.97
D8	678.80	104.95	997.44	465.11
D9	678.80	251.09	996.56	612.13
D10	678.80	174.03	1001.92	529.71

[a] The value is from Ref[2]; [b] At the B3LYP/aug-cc-pVTZ level; [c] The value is from Ref[3]; [d] The value is from Ref[4].

Table S4. Predicted entropies (S_{salt}), entropies of reaction ($\triangle S_{rxn}$), enthalpies of reaction ($\triangle H_{rxn}$), and free energies of reaction ($\triangle G_{rxn}$) of the salts.

Anion	S_{salts}	ΔS_{rxn}	ΔH_{rxn}	ΔG_{rxn}
A1	276.19	-691.82	-432.22	-226.06
A2	285.54	-693.82	-377.04	-170.28
A3	296.46	-731.87	-400.48	-182.39
A4	293.78	-708.75	-437.10	-225.89
A5	301.19	-715.84	-429.20	-215.88
A6	391.20	-860.75	-309.18	-52.68
A7	399.75	-872.18	-263.69	-3.78
A8	414.02	-885.93	-279.08	-15.08
A9	408.29	-880.03	-318.55	-56.30
A10	418.77	-881.39	-317.63	-54.97
B1	291.98	-695.01	-464.75	-257.63
B2	302.44	-715.09	-438.67	-225.57
B3	312.09	-761.65	-466.74	-239.77
B4	305.94	-742.85	-494.29	-272.92
B5	316.42	-751.01	-485.64	-261.84
B6	403.00	-883.34	-348.31	-85.08
B7	415.57	-899.15	-323.99	-56.04
B8	427.93	-928.01	-340.17	-63.63
B9	423.28	-914.07	-368.50	-96.11
B10	426.23	-911.47	-358.74	-87.12
C1	335.20	-788.18	-443.03	-208.16
C2	346.27	-807.48	-445.82	-205.19
C3	362.99	-821.64	-415.18	-170.33
C4	363.04	-792.74	-433.93	-197.69
C5	363.76	-828.79	-452.83	-205.85
C6	463.35	-959.30	-319.71	-33.83
C7	472.18	-965.13	-334.90	-47.29
C8	475.53	-986.16	-322.10	-28.23
C9	478.91	-983.29	-337.52	-44.50
C10	484.04	-996.58	-339.82	-42.83
D1	388.74	-868.05	-428.31	-169.63
D2	401.90	-873.65	-441.33	-180.98
D3	413.32	-919.82	-462.59	-188.49
D4	408.93	-898.29	-441.32	-173.63
D5	414.67	-915.87	-435.54	-162.61

D6	500.83	-1033.40	-347.35	-39.40
D7	517.25	-1056.83	-351.61	-36.68
D8	529.85	-1069.37	-351.33	-32.65
D9	530.92	-1067.02	-342.02	-24.05
D10	524.45	-1091.43	-350.23	-24.98

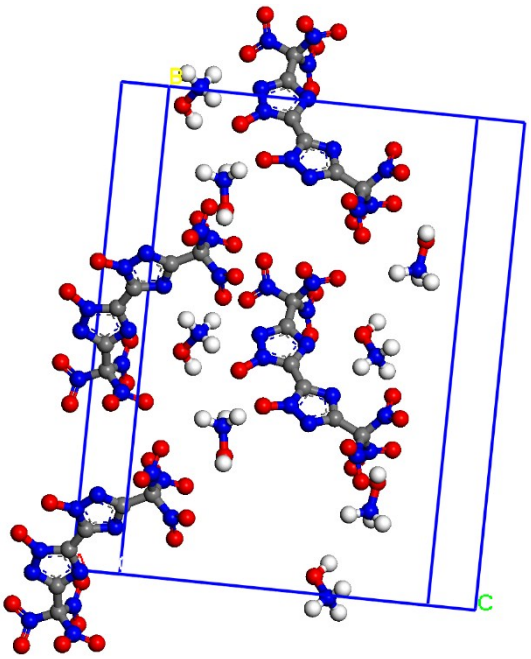


Figure S1. Optimized crystal structure of the **B6**

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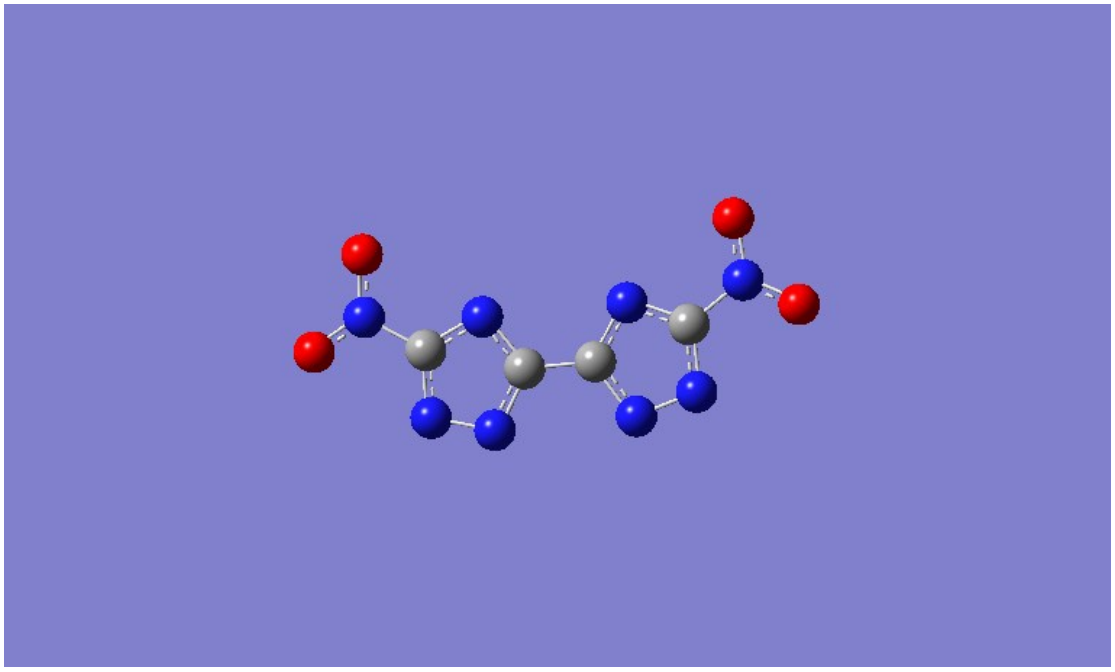

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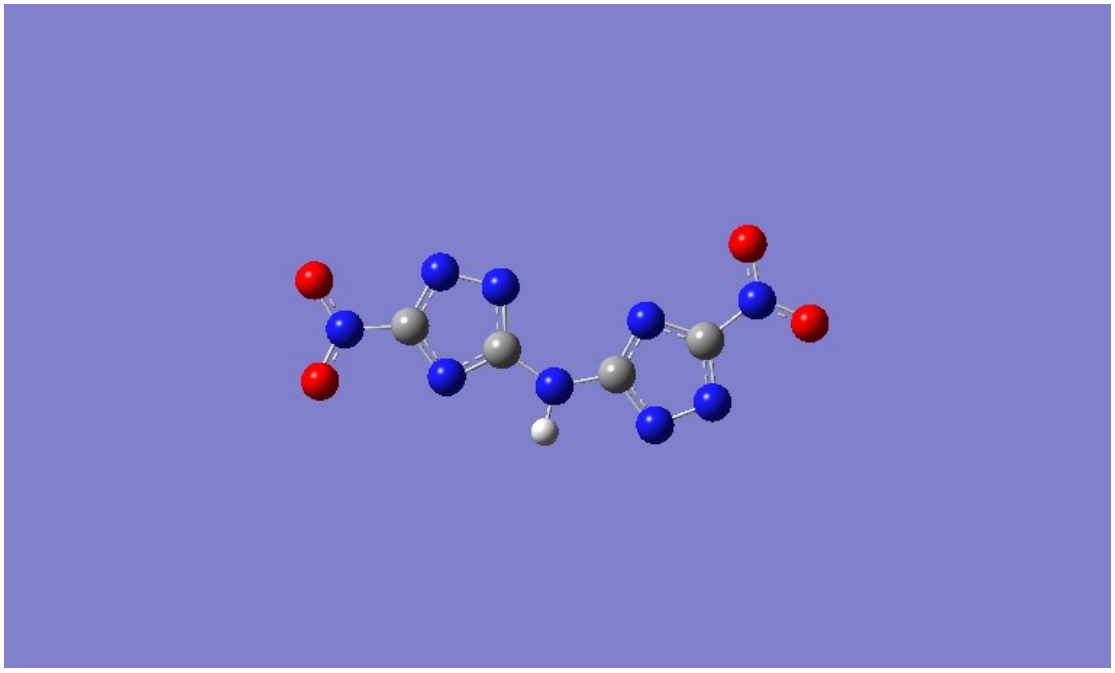

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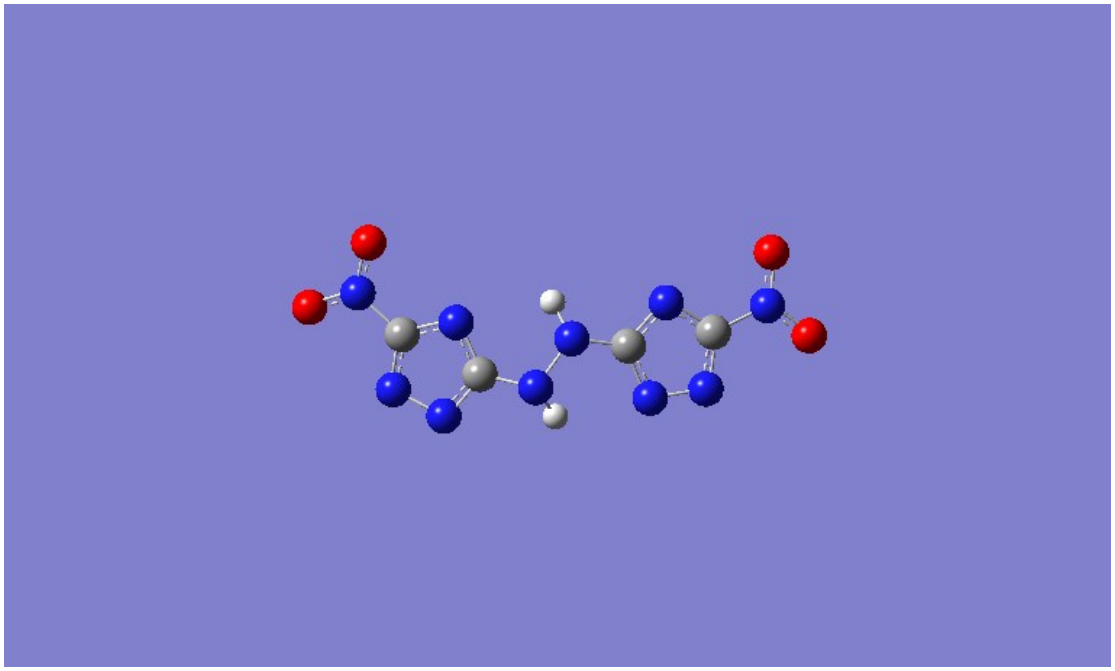

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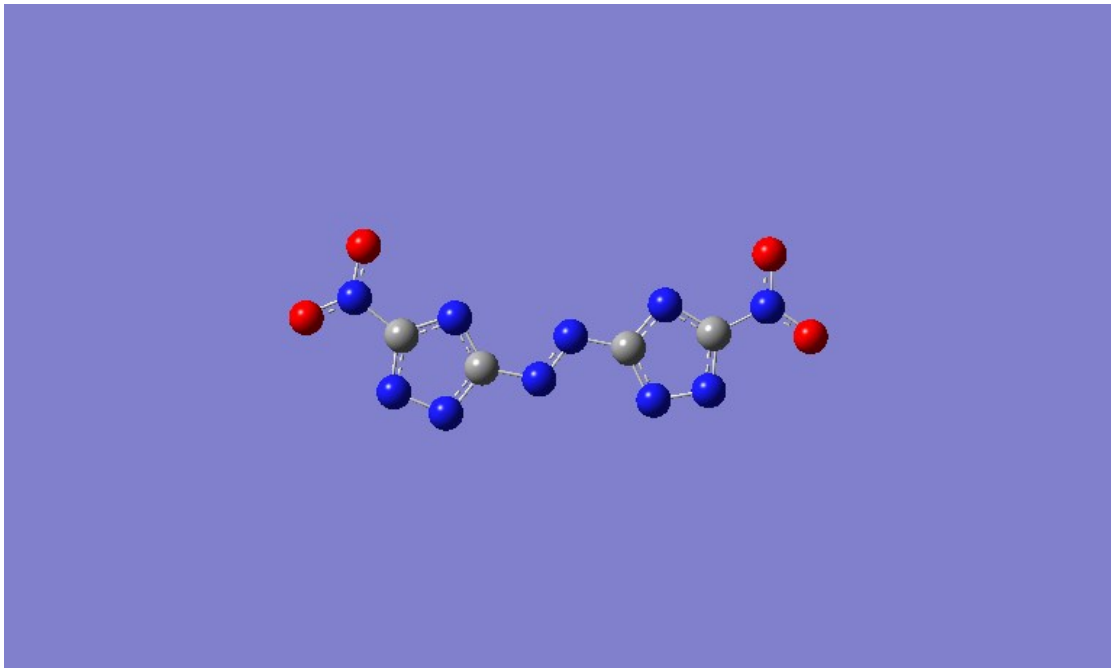

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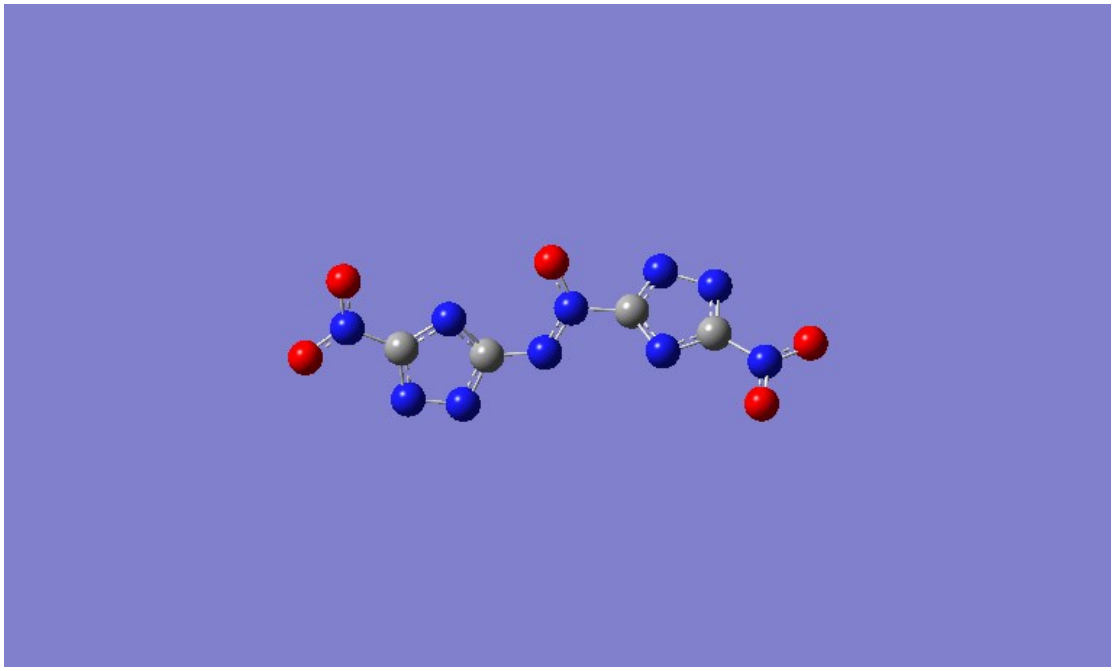

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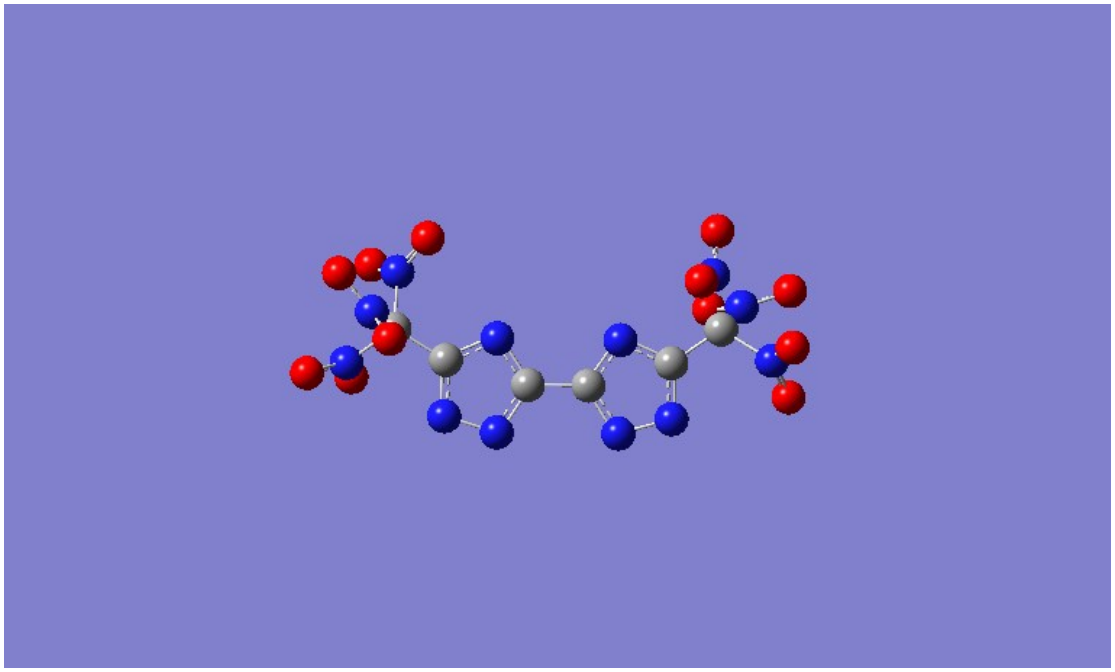

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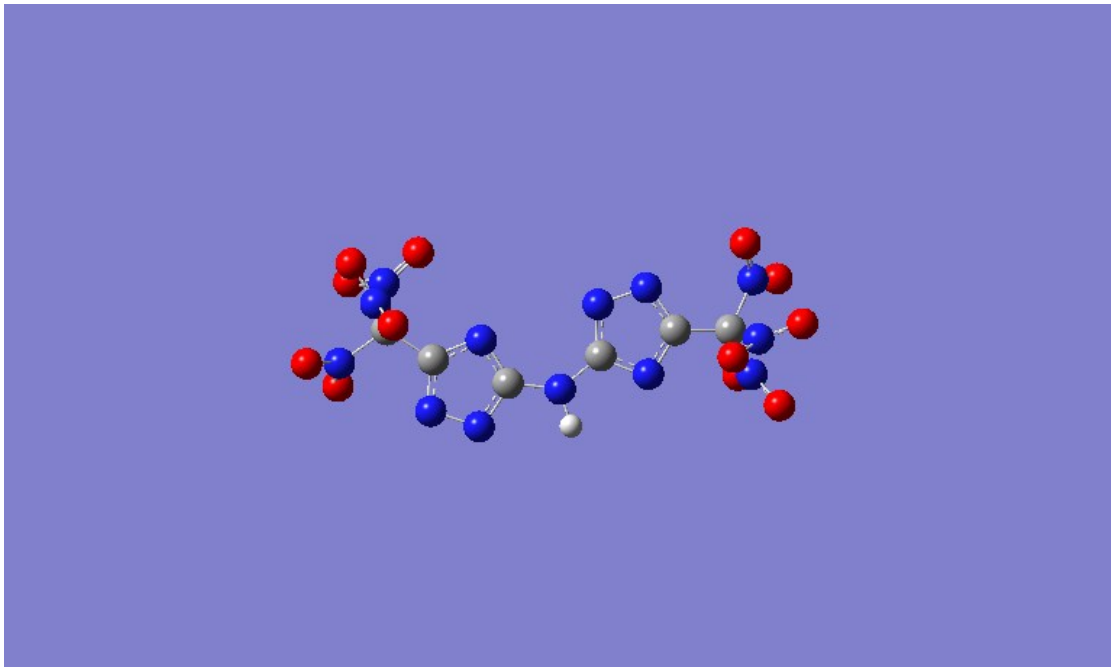

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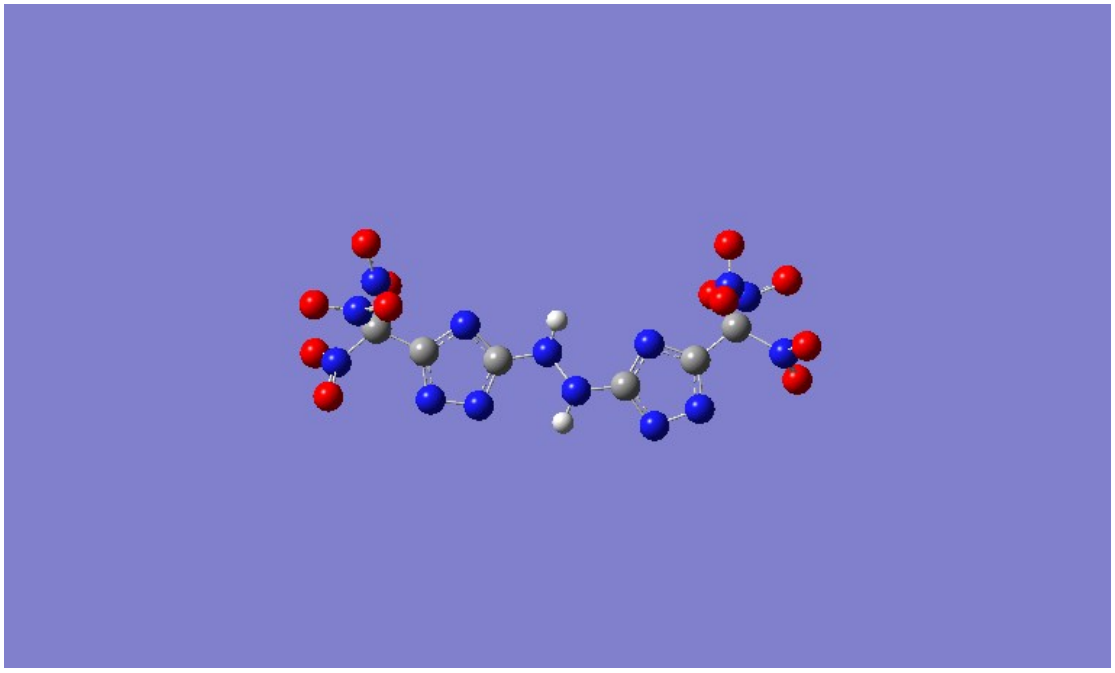

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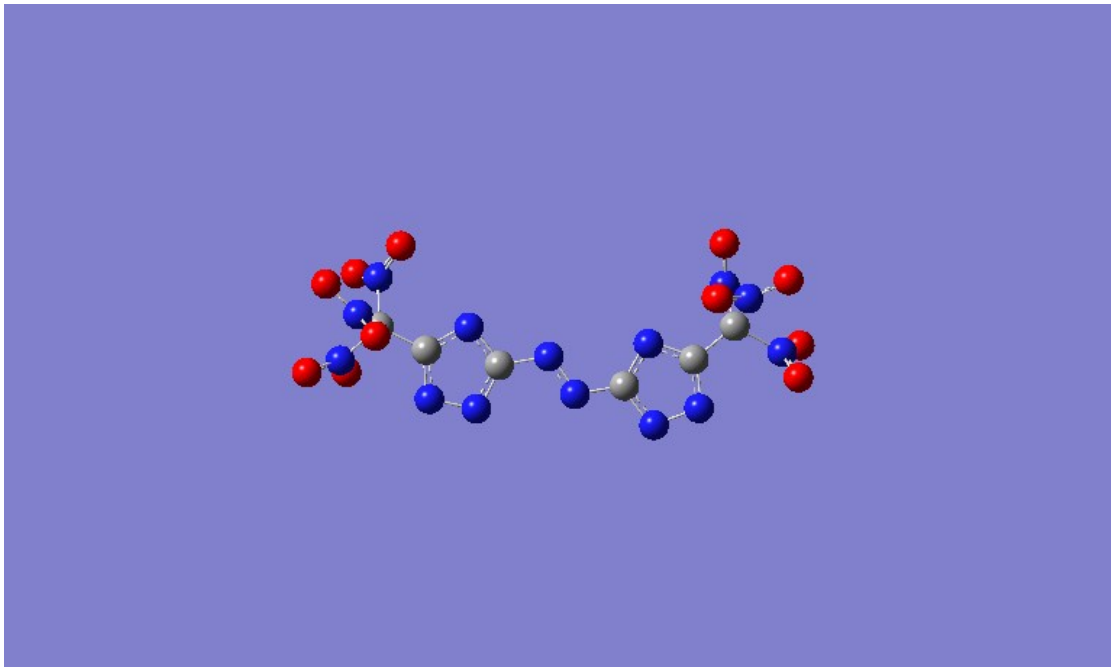

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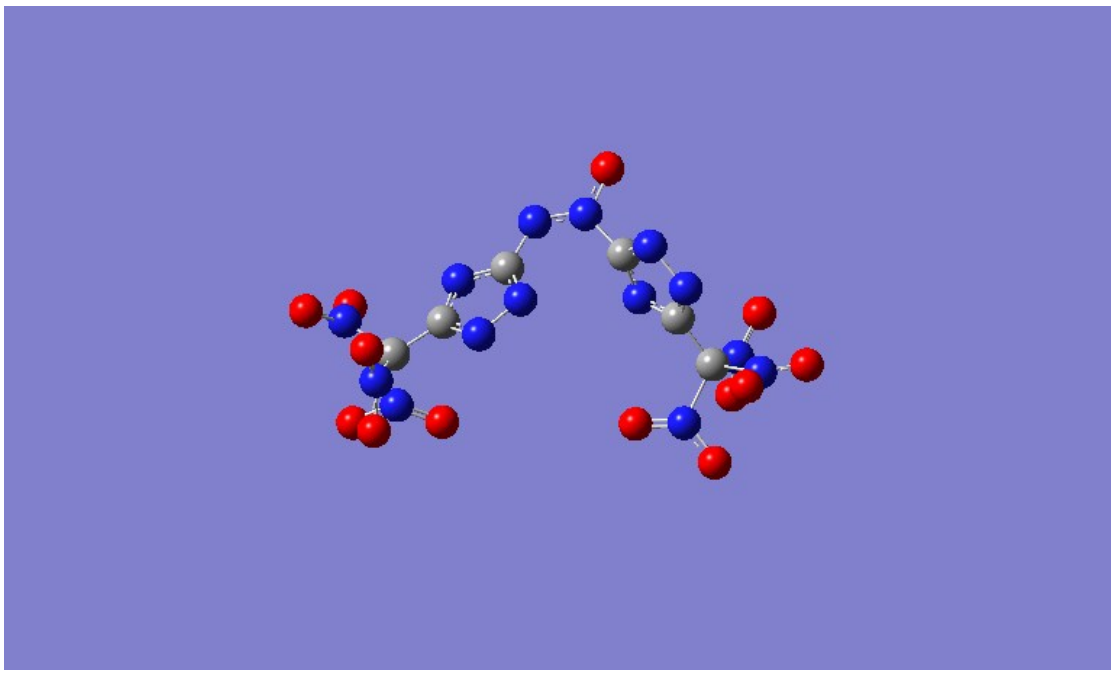

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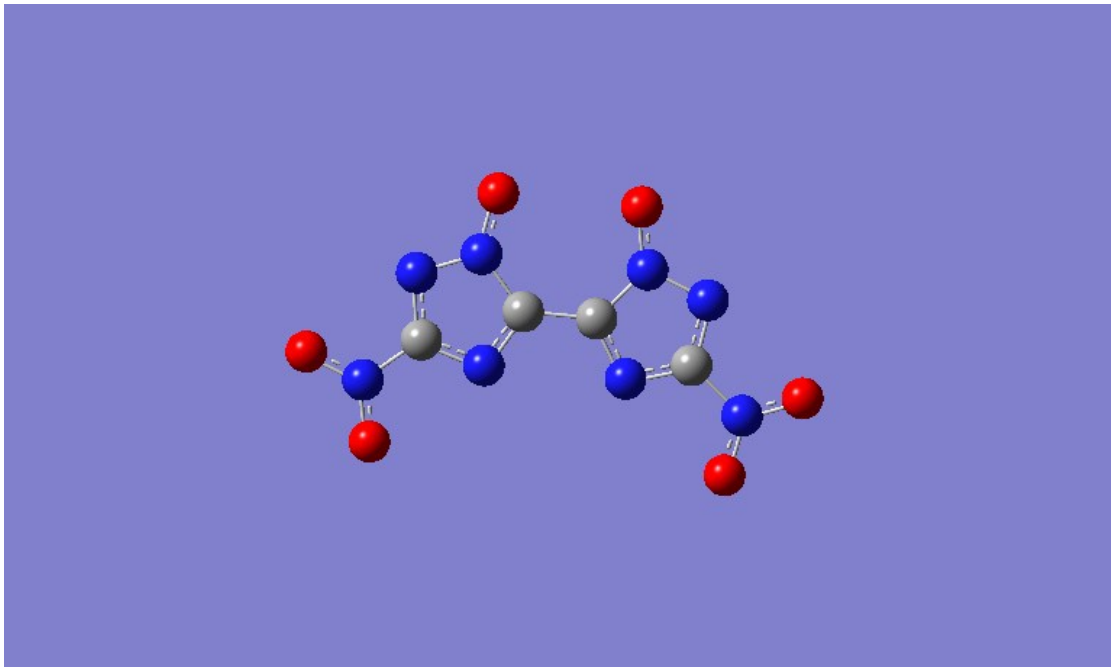

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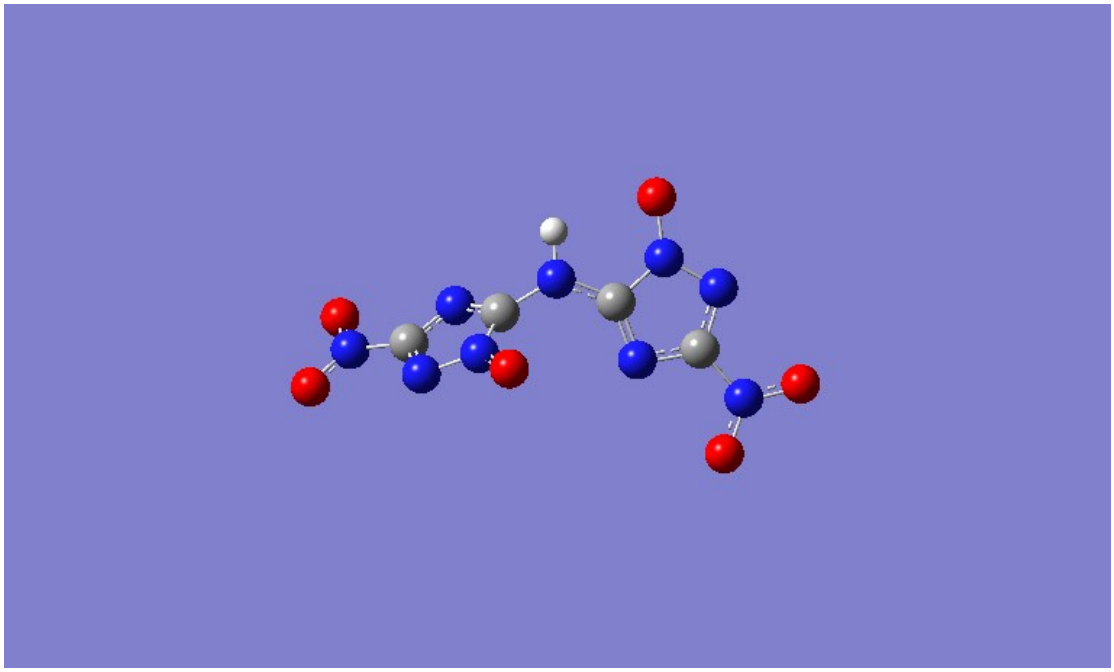

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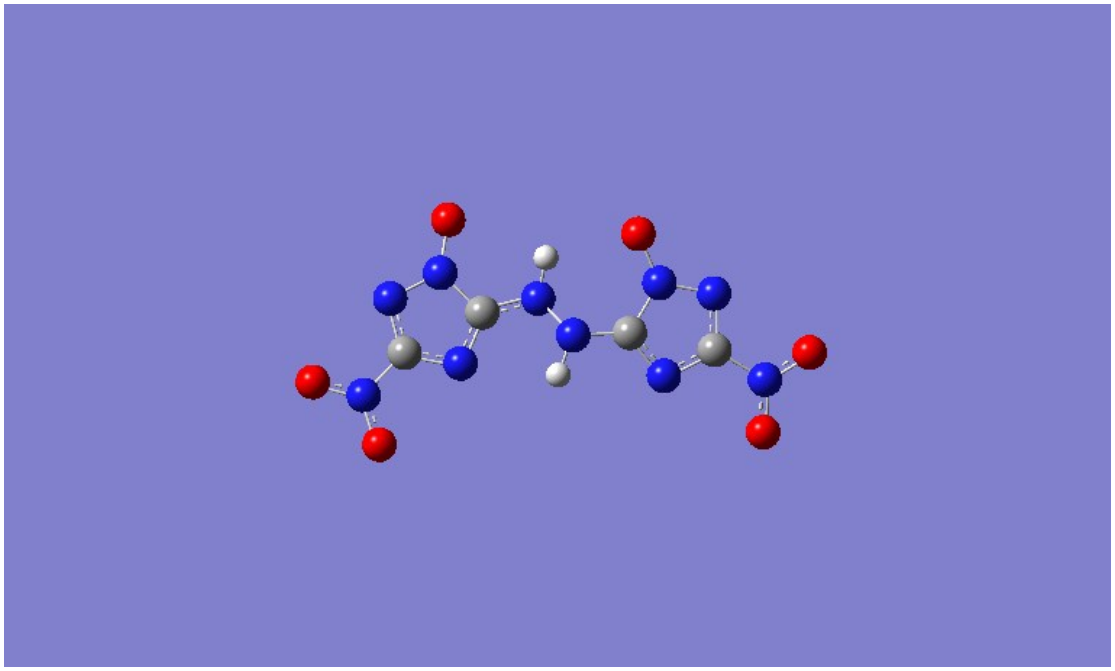

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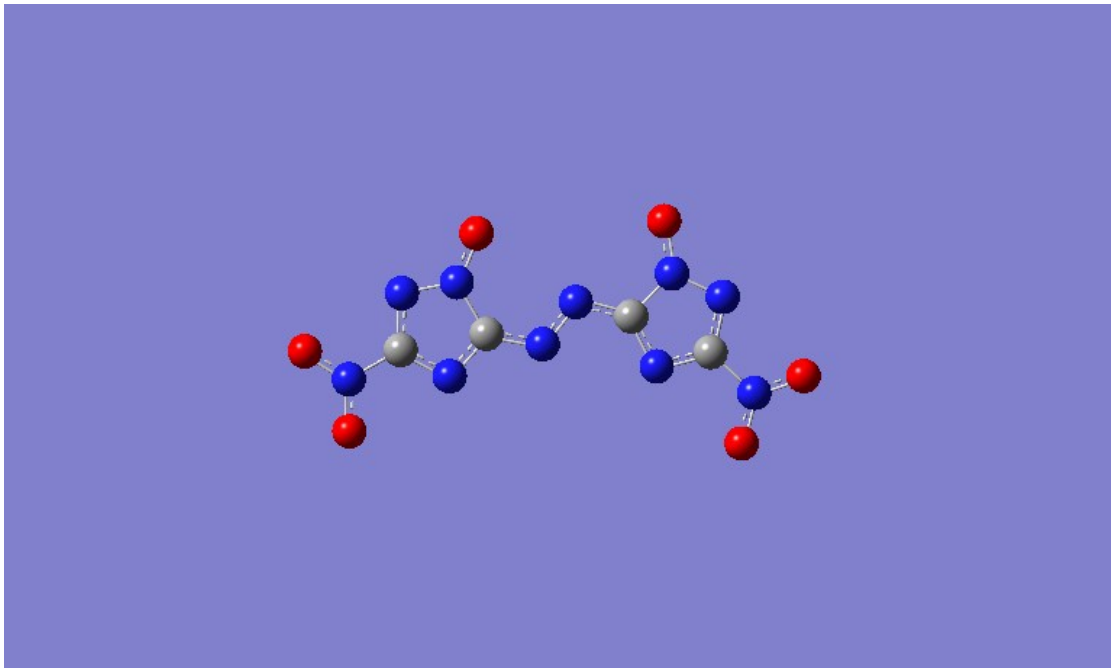

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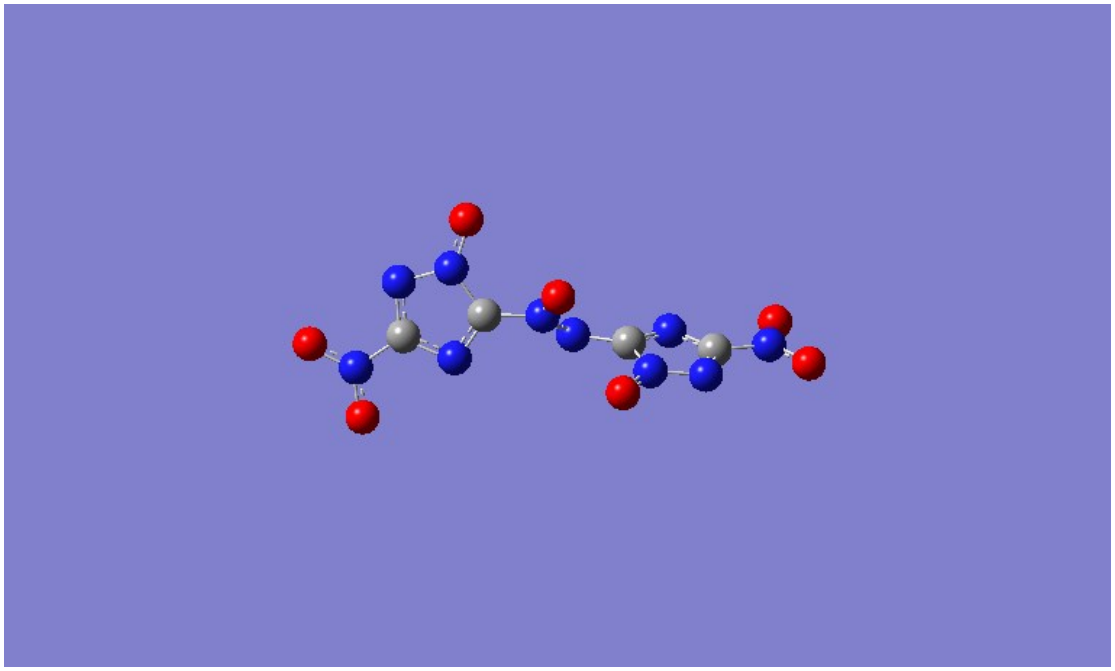

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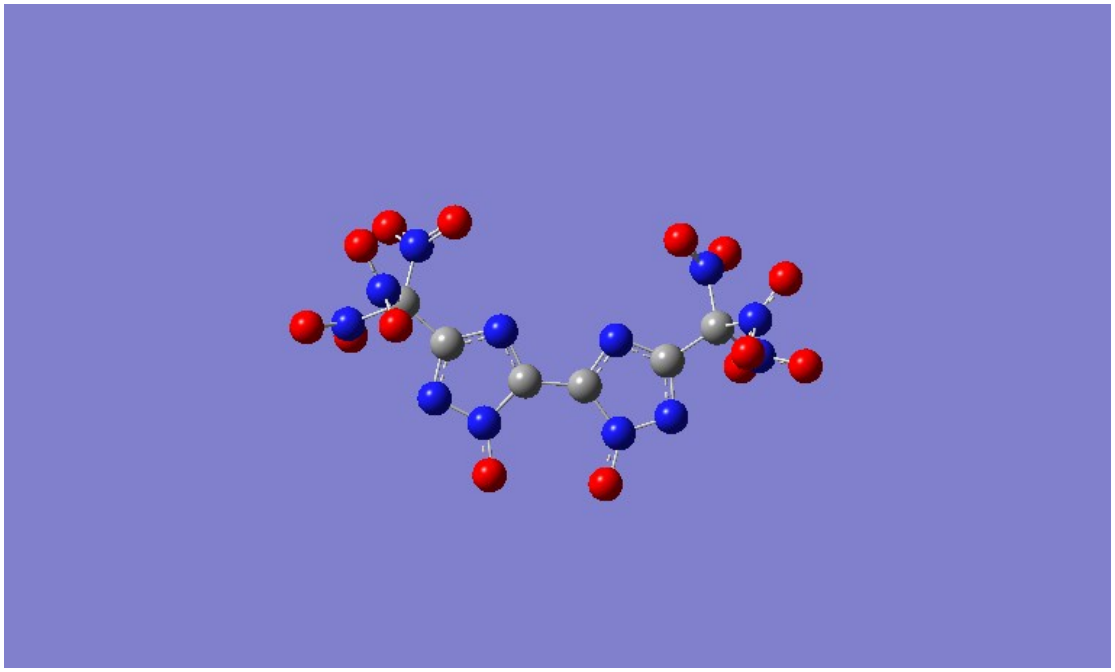

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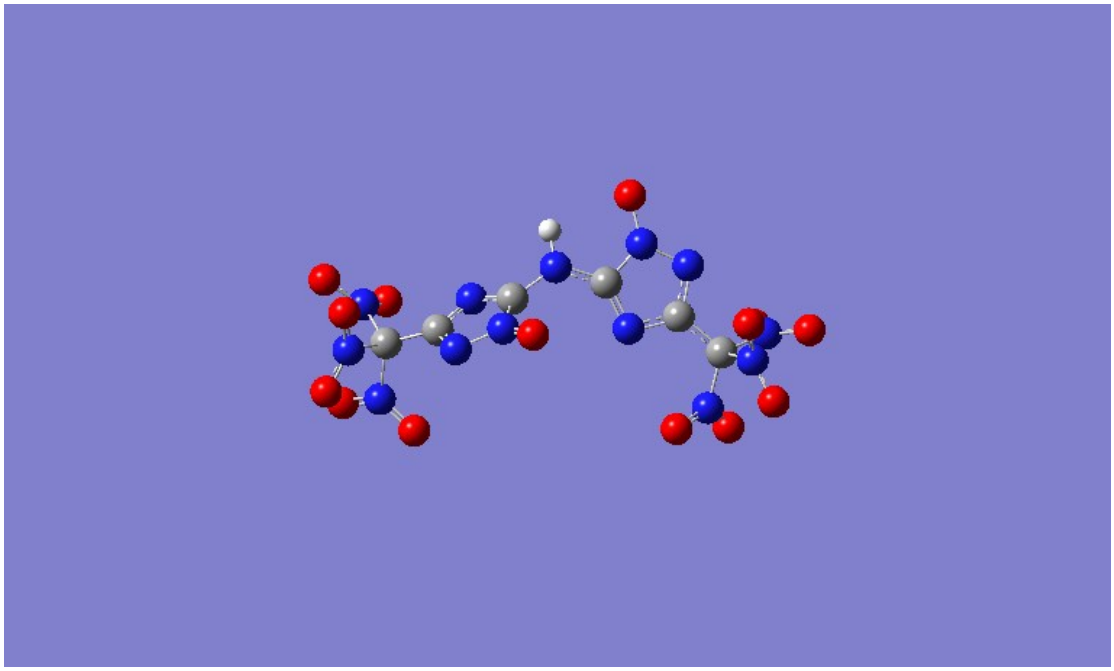

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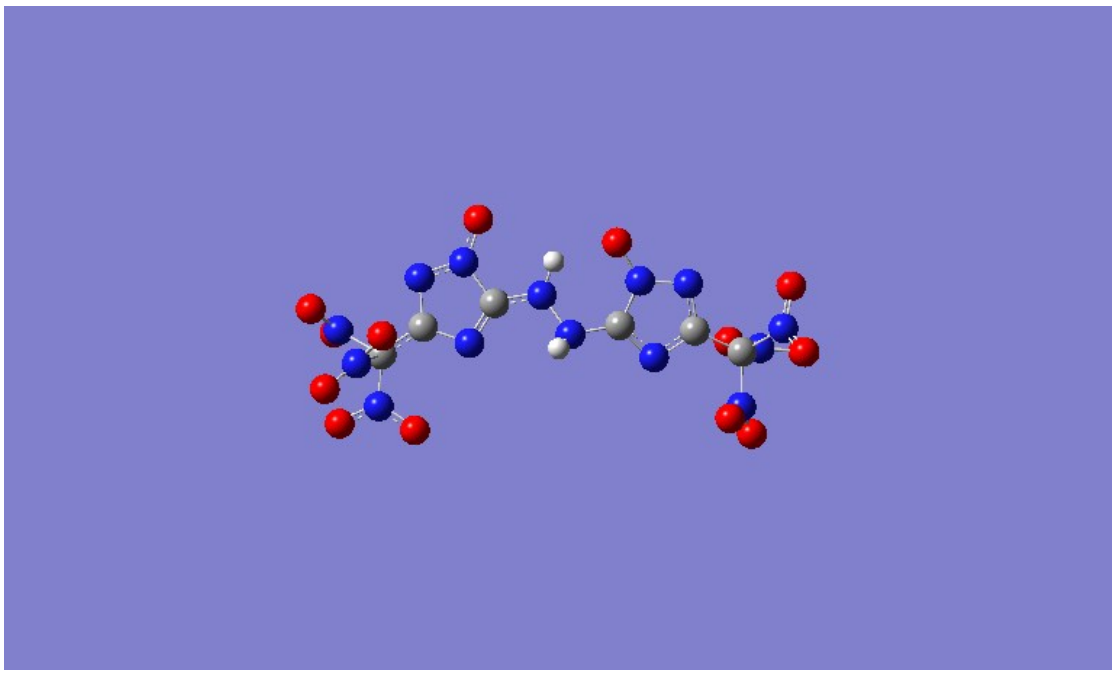

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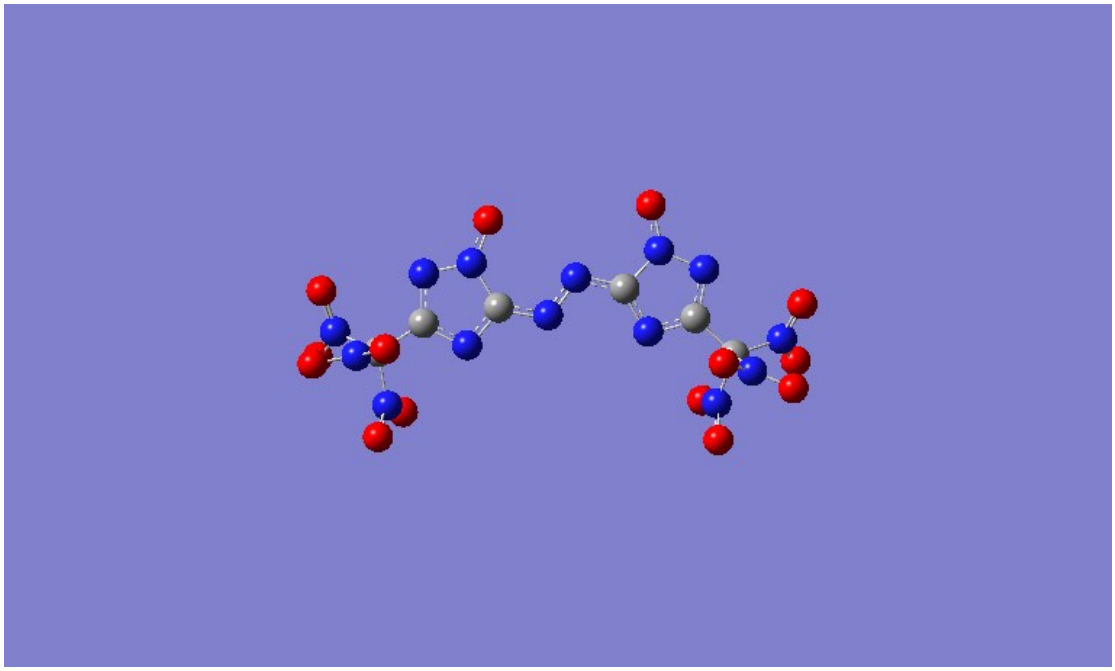

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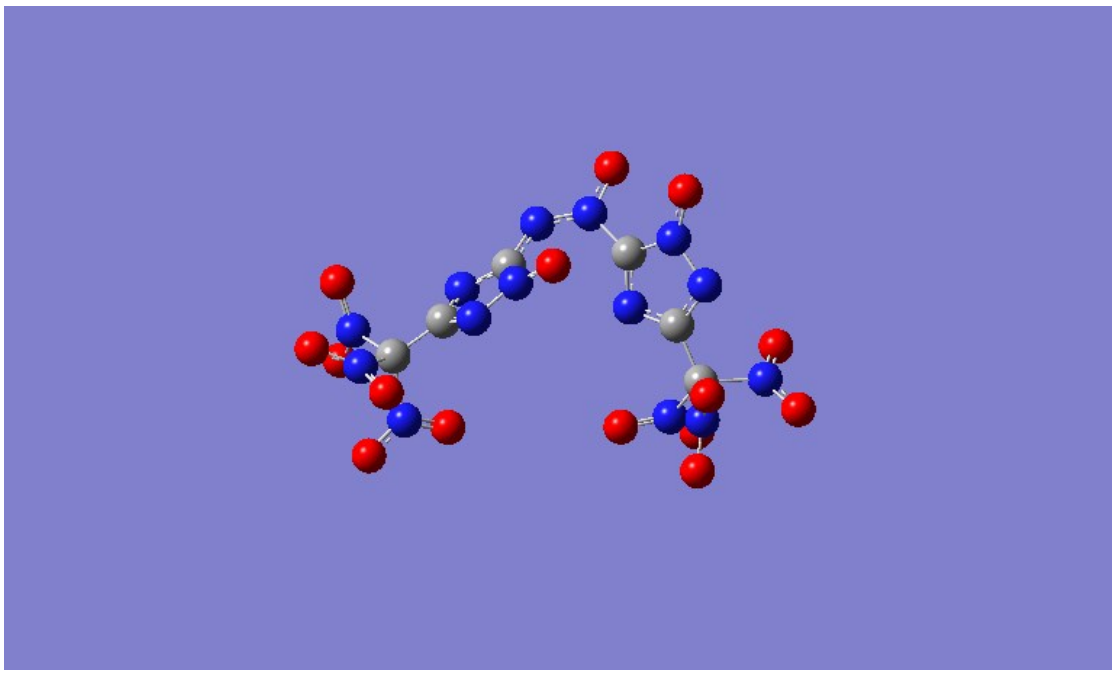

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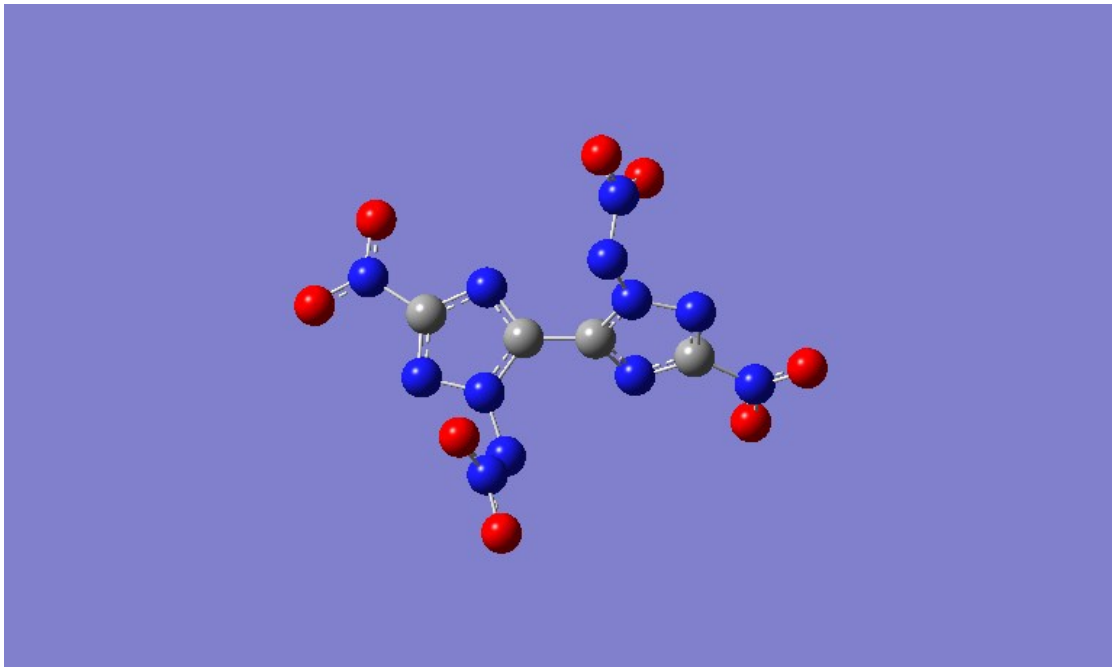

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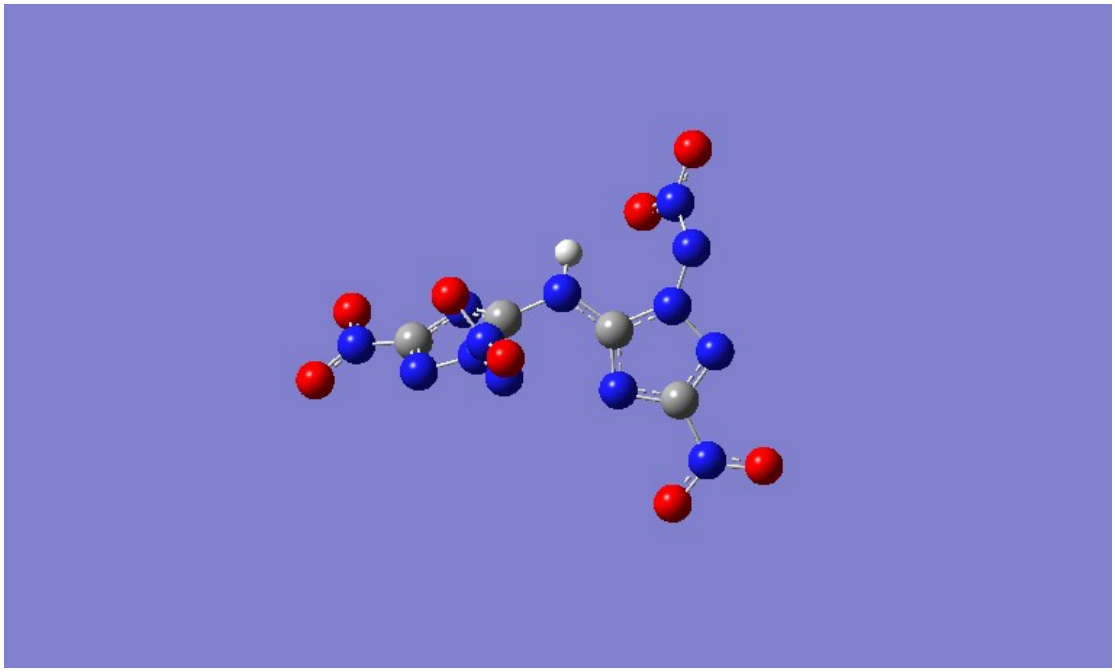

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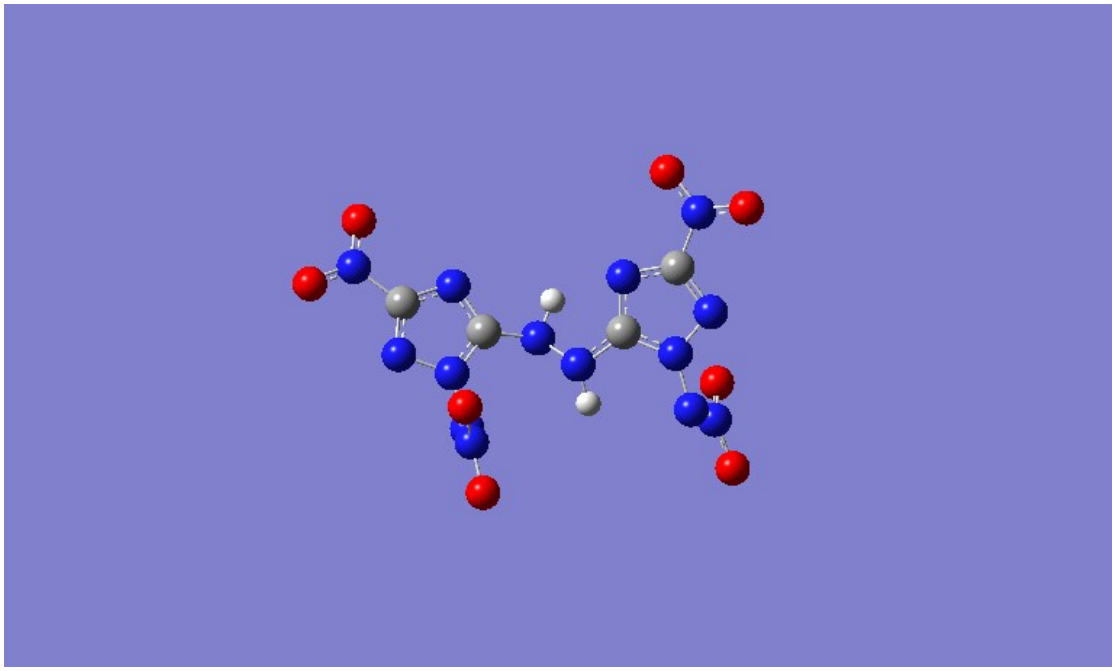

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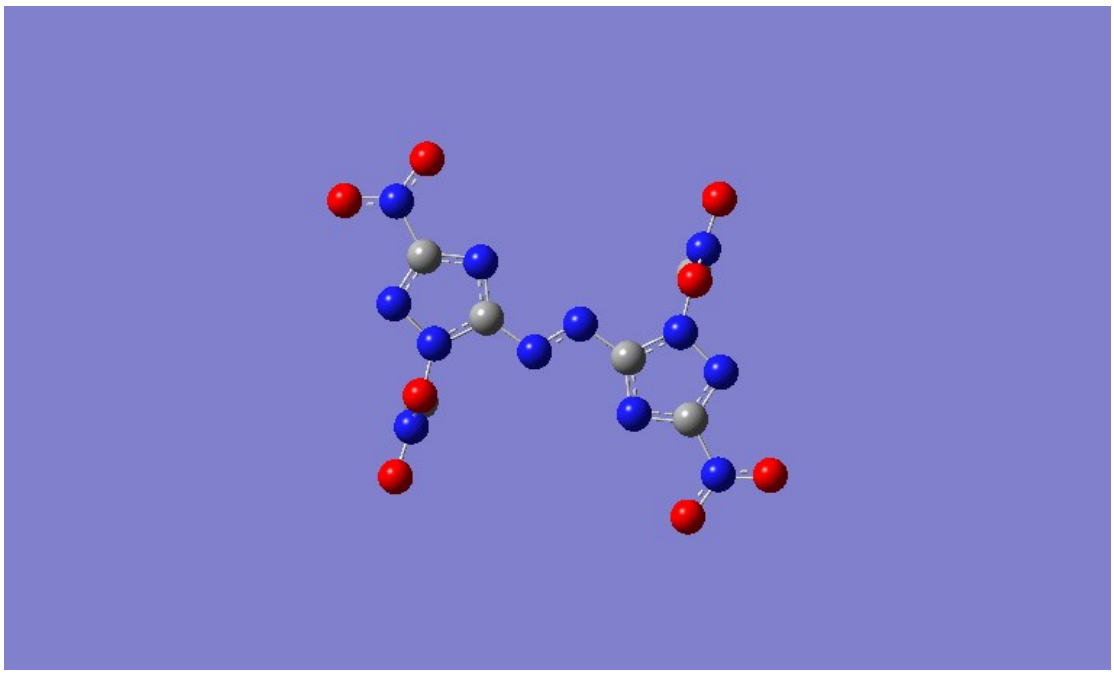

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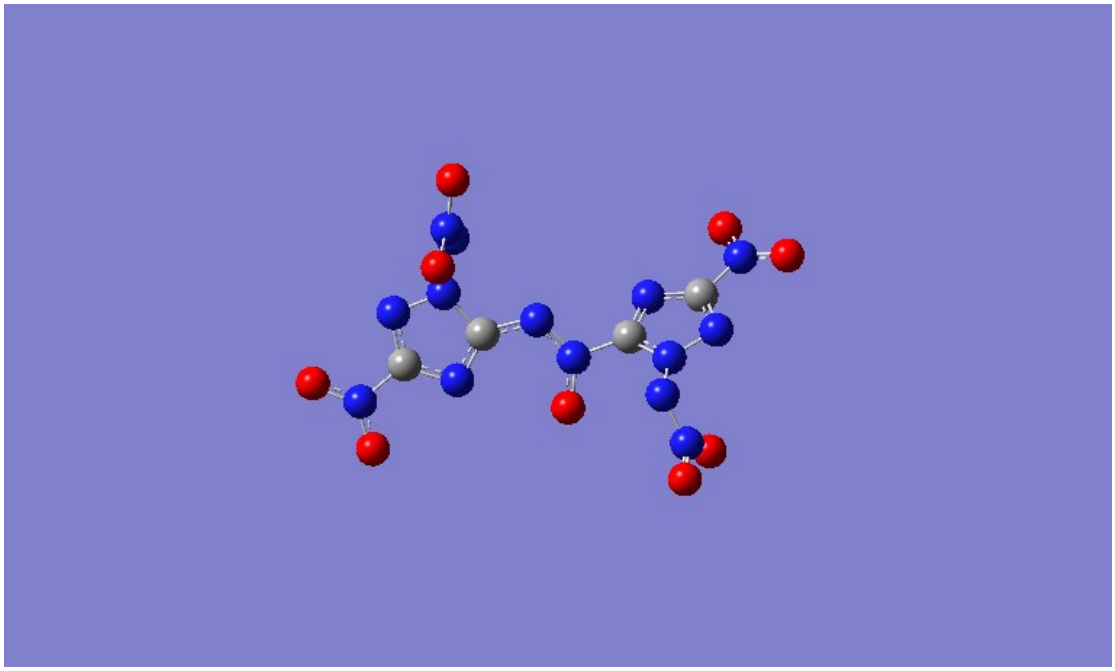

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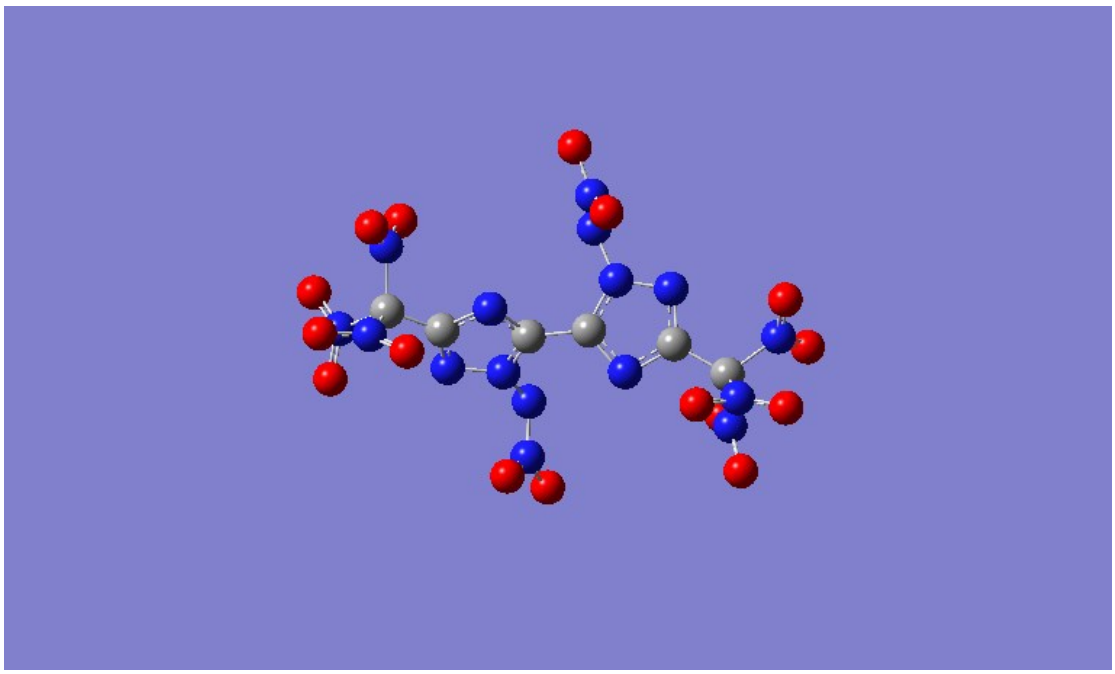

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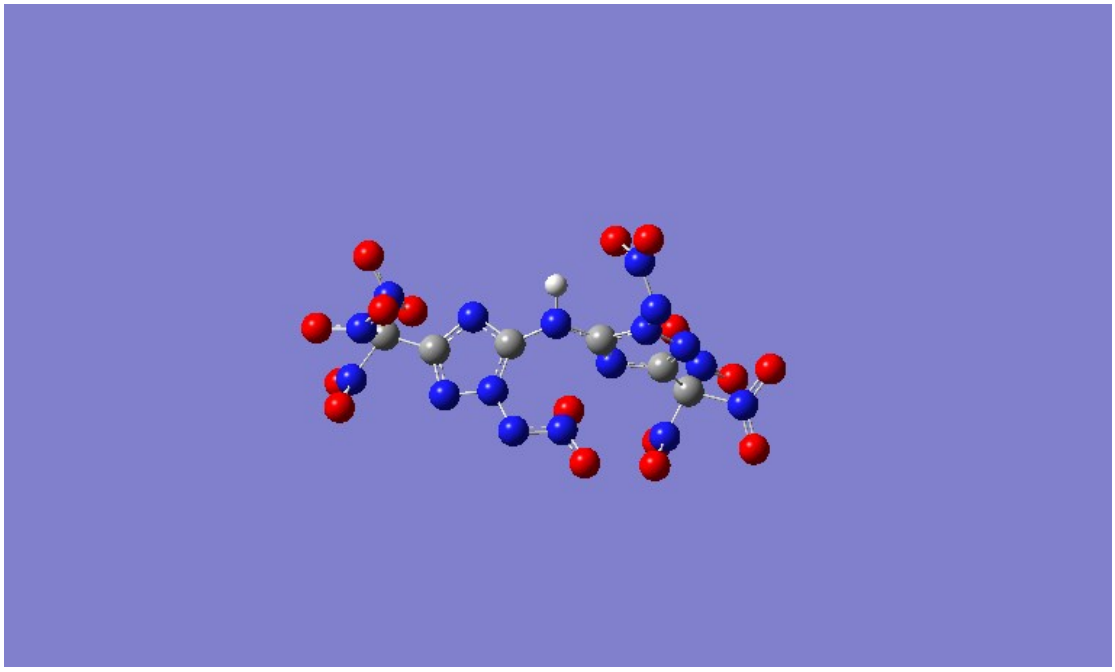

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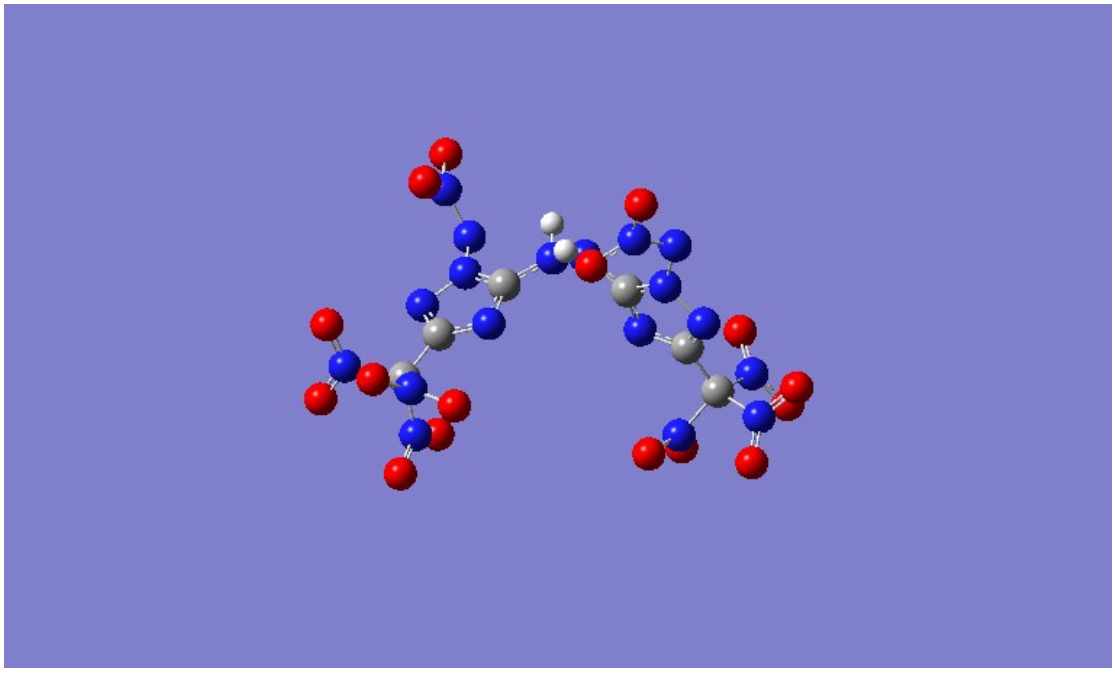

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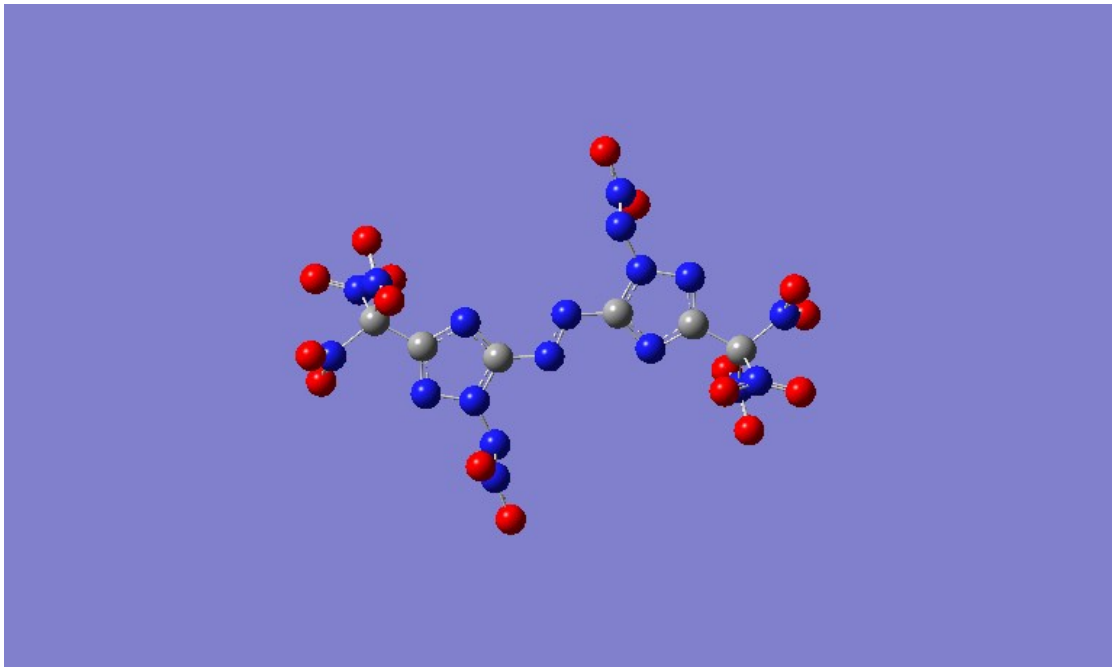

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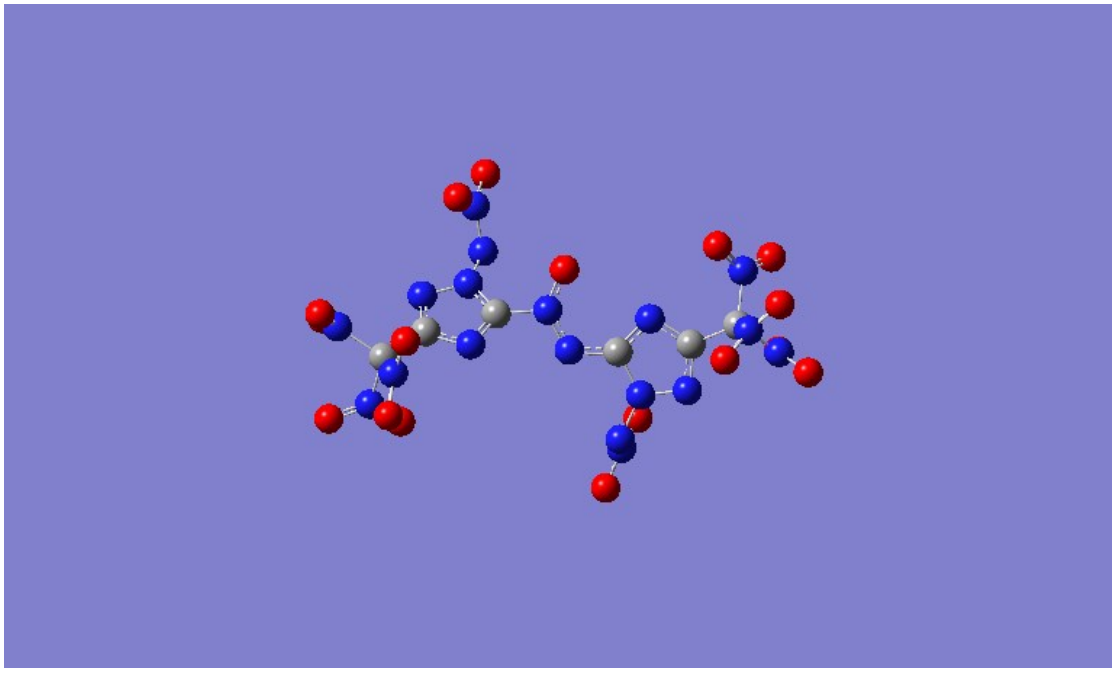

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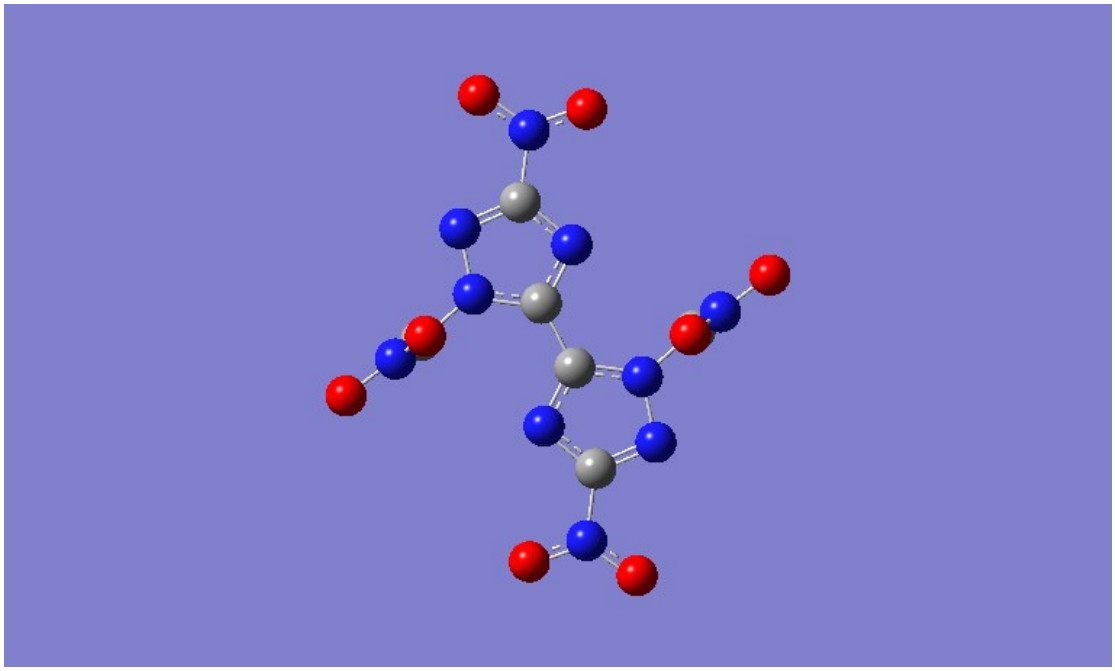

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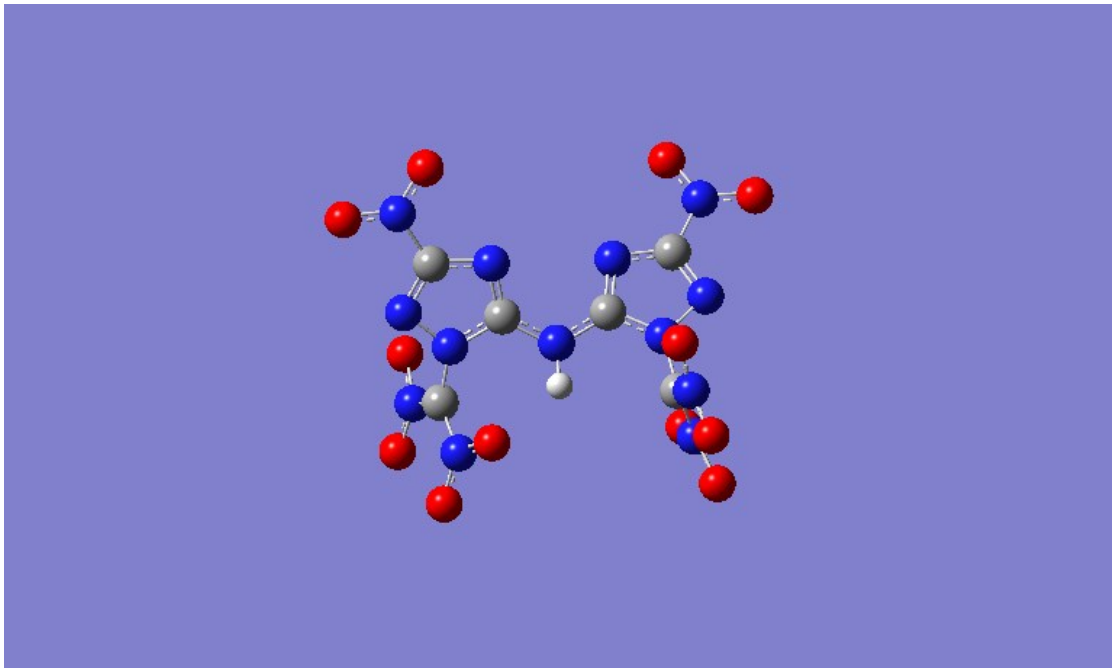

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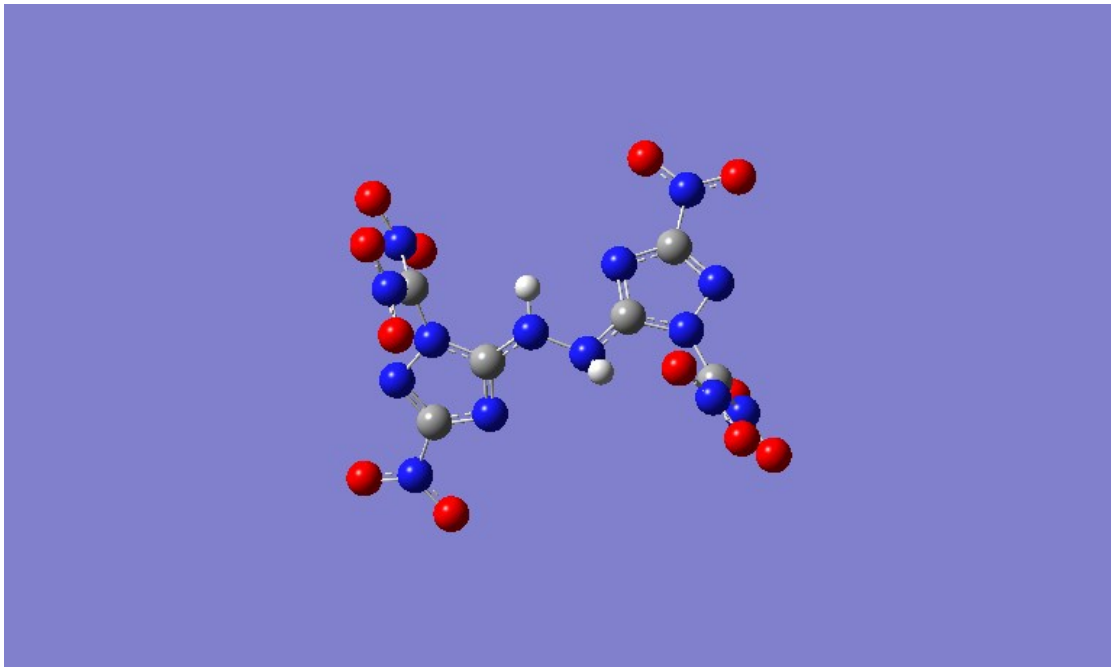

Anion D4

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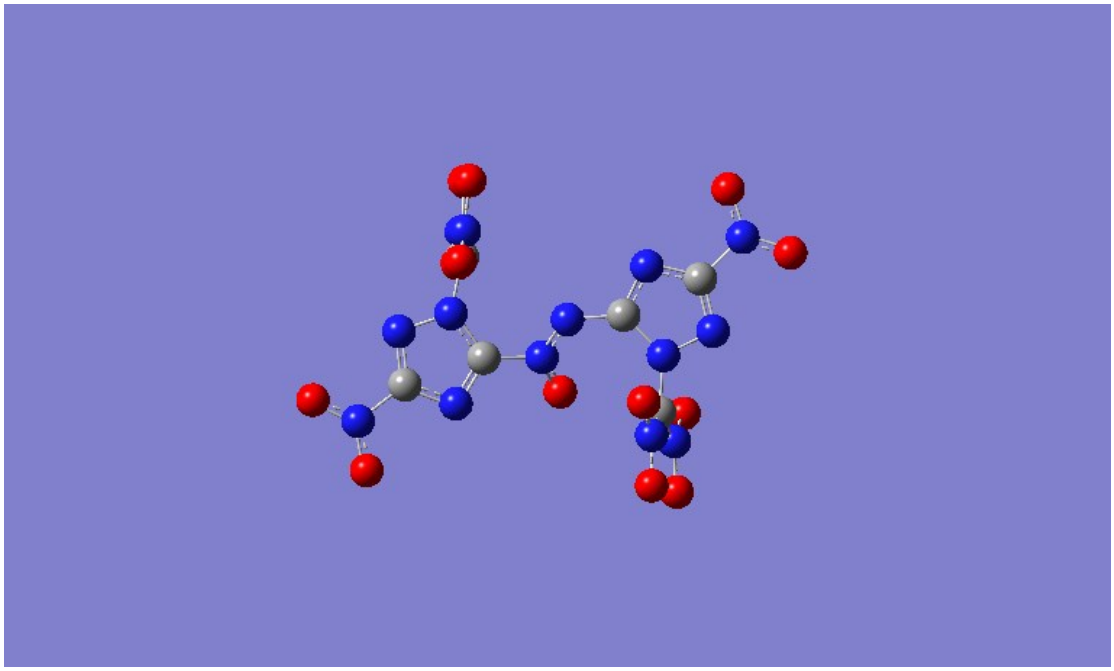

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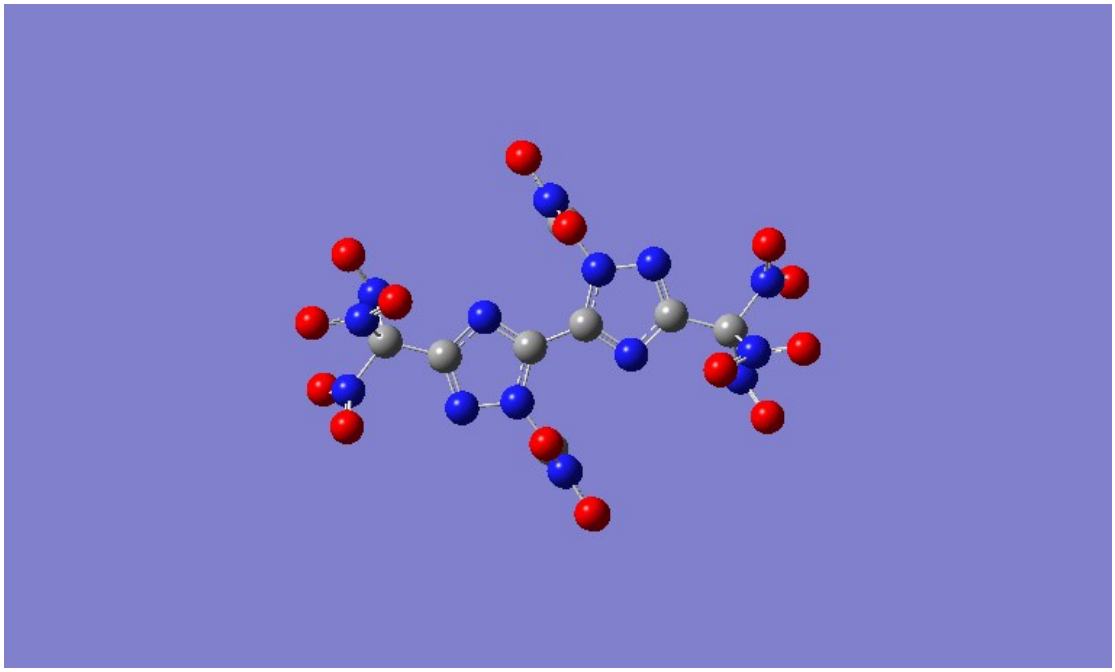

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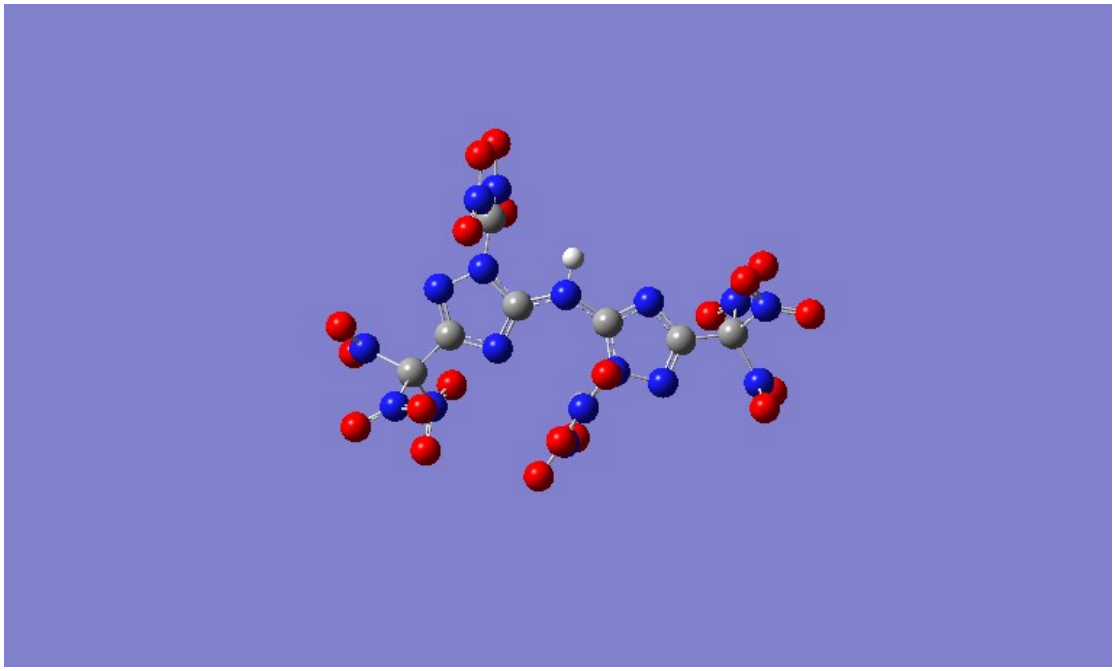

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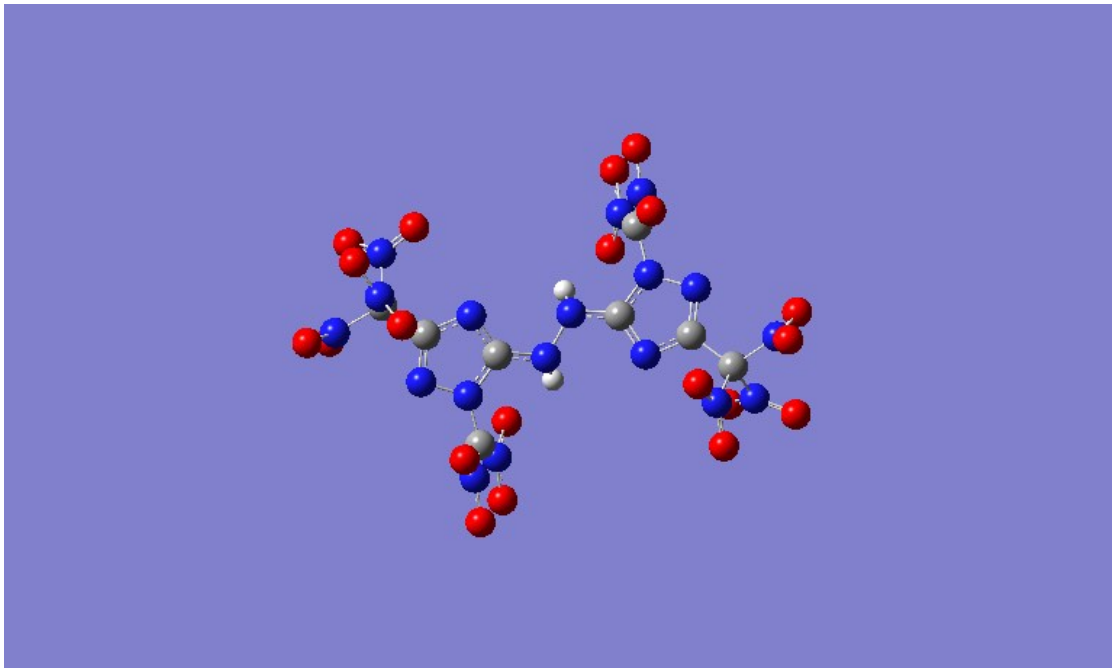

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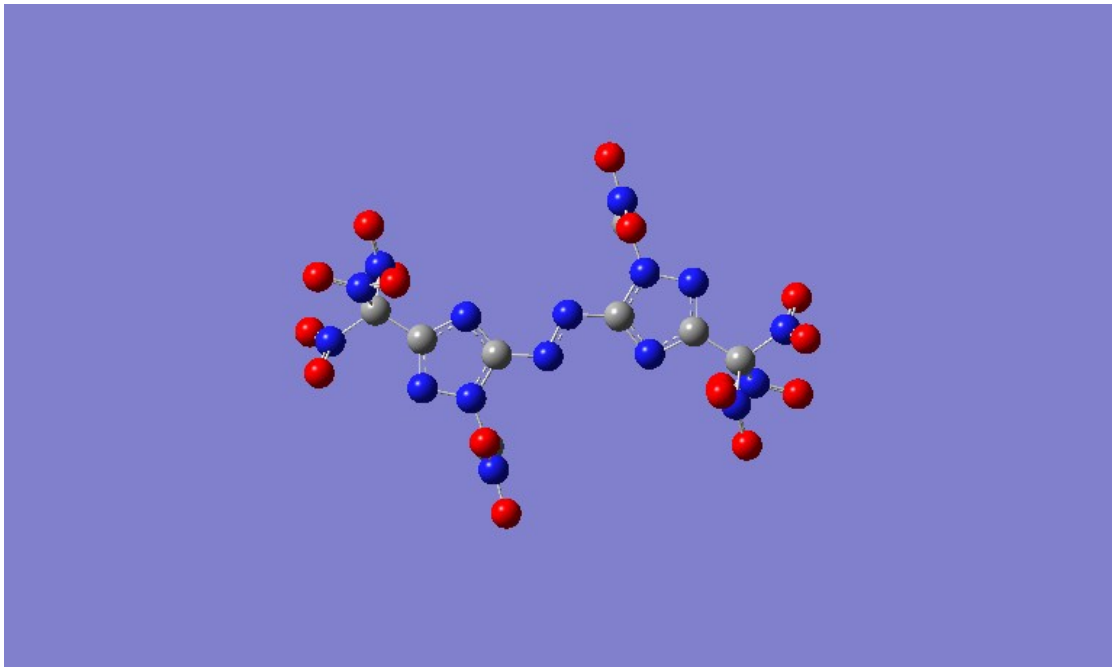

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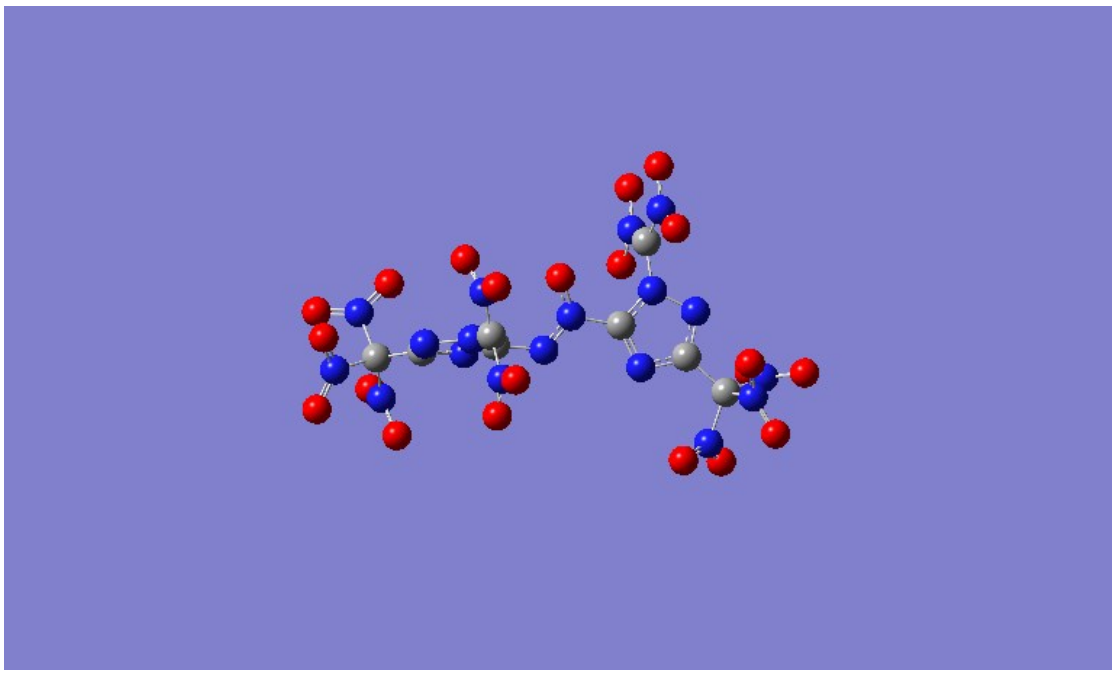

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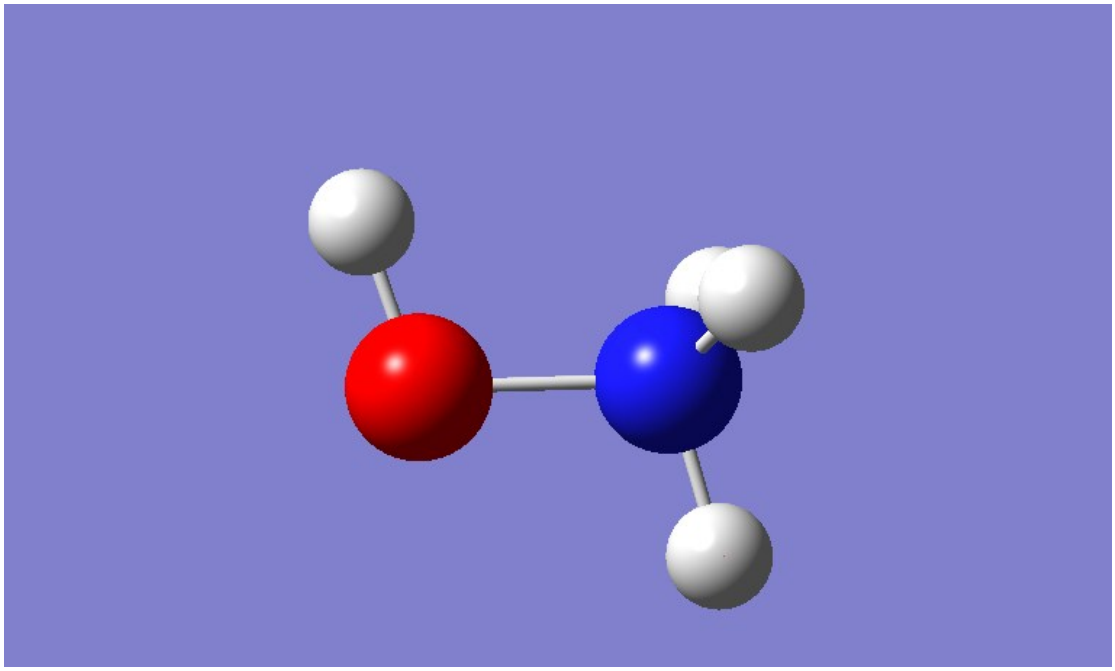

Figure S1. Optimized structures of the related anions and cation

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