Supporting Information

Combined Computational and Experimental Study on Designing Balanced Tetrazole-Based Energetic Materials

Hao Li [b], Wen-Zhu Zu [a], Xiao-Yu Fan, [a] Qian Zhang [*a], Yan Huang [*a]

[a] School of Chemistry and Chemical Engineering Huanggang Normal University, Huanggang 438000, China

[b] Xi'an North Qinghua Electromechanical Group Co., Ltd., Xi'an 710025, China.

content

Part I DFT calculational study details

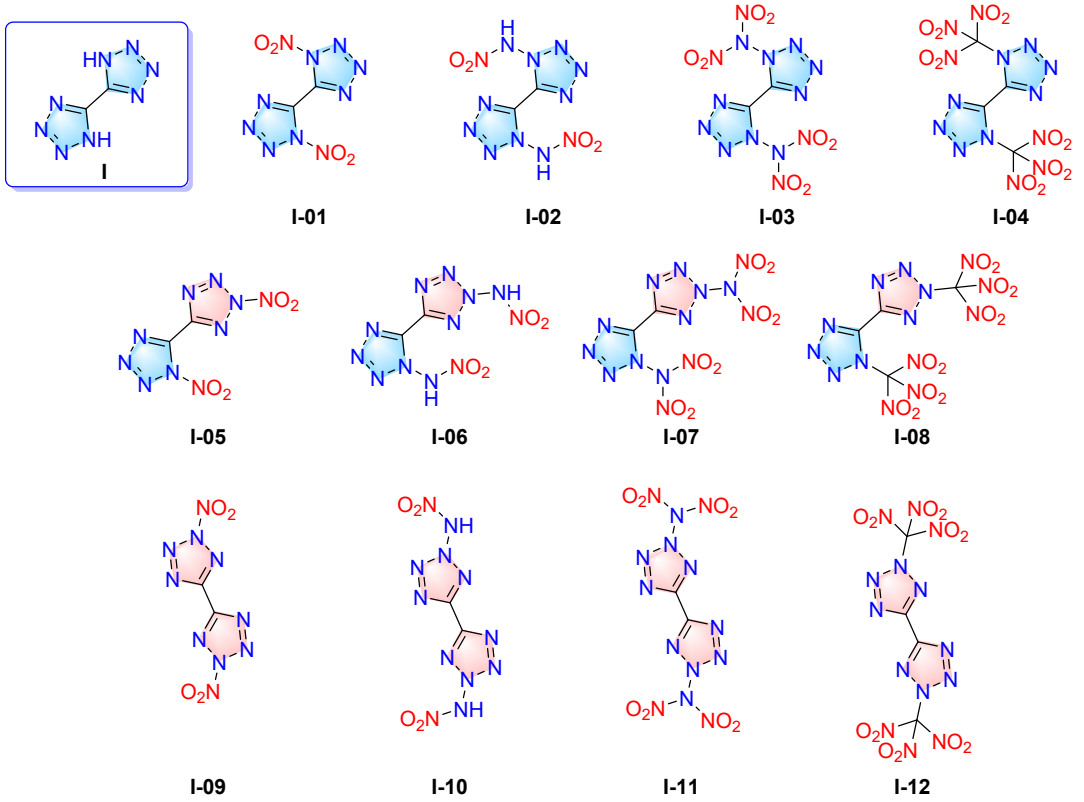


Fig. **S1** Structure of series **I** designed molecules

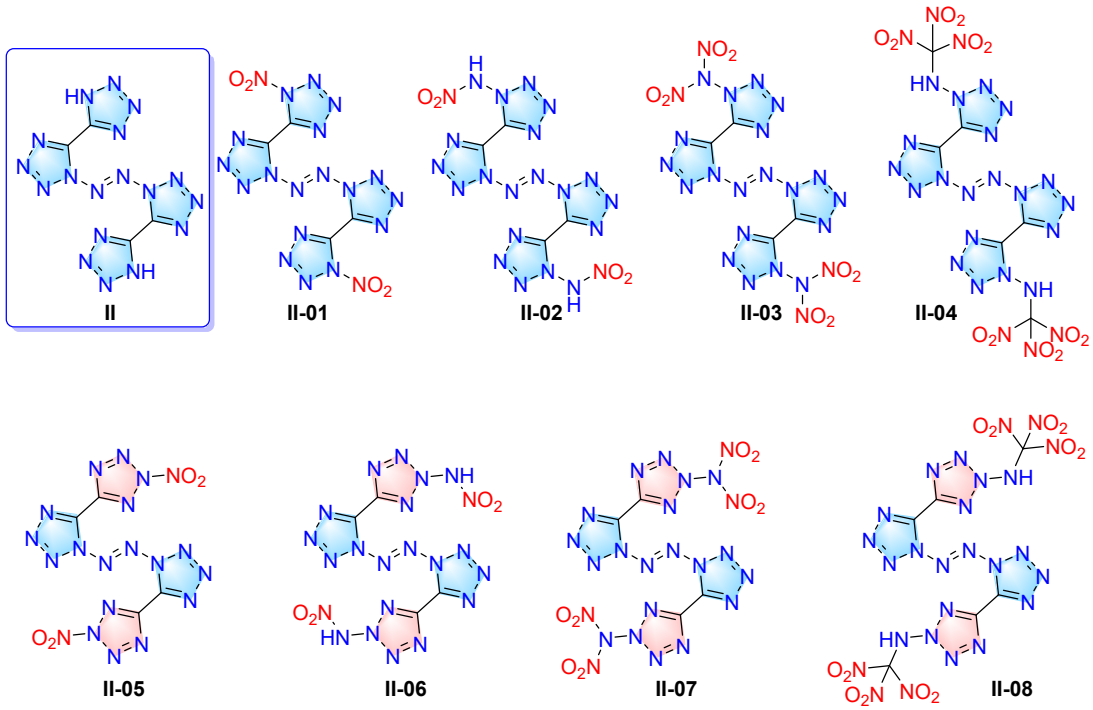
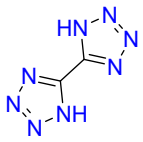
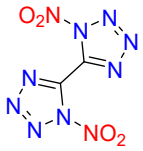


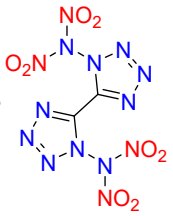
Fig. **S2** Structure of series **II** designed molecules

I  + 2 CH_4 ⟶ 2  + CH_3CH_3

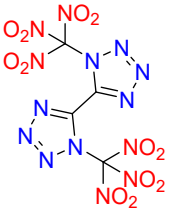
I-01  + 2 CH_4 + 2 NH_3 ⟶ 2  + 2 NH_2NO_2 + CH_3CH_3

I-02  + 2 CH_4 + 4 NH_3 ⟶ 2  + 2 NH_2NO_2

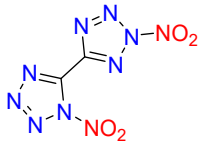
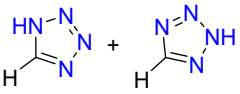
+ 2 NH_2NH_2 + CH_3CH_3

I-03  + 2 CH_4 + 6 NH_3 ⟶ 2  + 4 NH_2NO_2

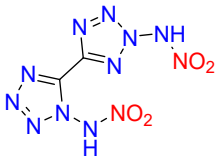
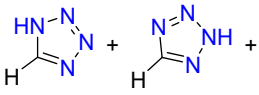
+ 2 NH_2NH_2 + CH_3CH_3

I-04  + 8 CH_4 + 2 NH_3 ⟶ 2  + 6 CH_3NO_2

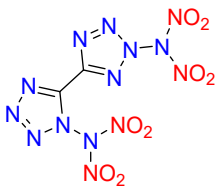
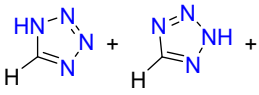
+ 2 CH_3NH_2 + CH_3CH_3

I-05  + 2 CH_4 + 2 NH_3 ⟶ 

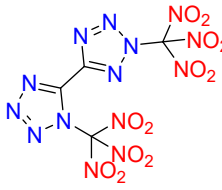
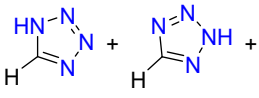
+ 2 NH_2NO_2 + CH_3CH_3

I-06  + 2 CH_4 + 2 NH_3 ⟶  + 2 NH_2NO_2

+ 2 NH_2NH_2 + CH_3CH_3

I-07  + 2 CH_4 + 6 NH_3 ⟶  + 4 NH_2NO_2

+ 2 NH_2NH_2 + CH_3CH_3

I-08  + 8 CH_4 + 2 NH_3 ⟶  + 6 CH_3NO_2

+ 2 CH_3NH_2 + CH_3CH_3

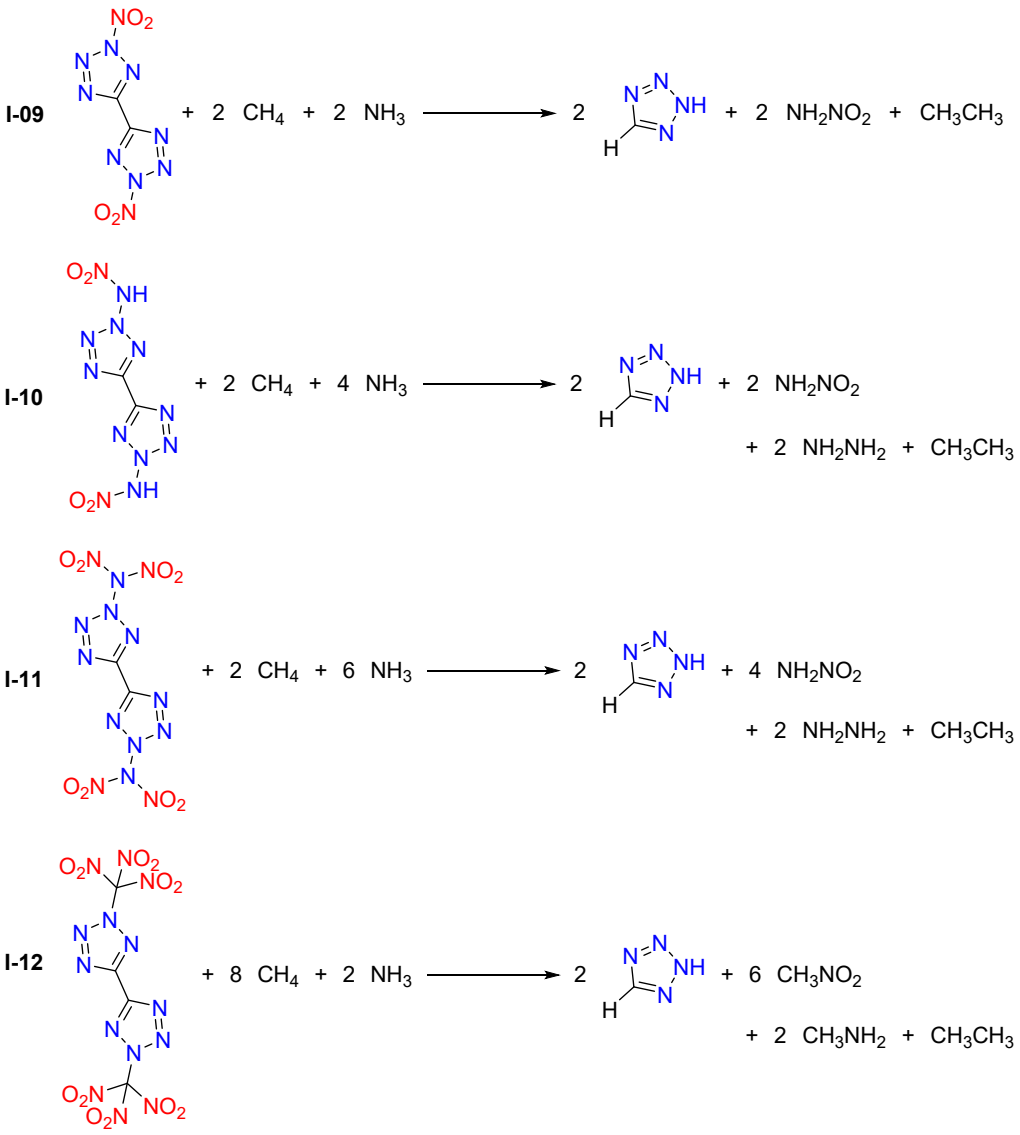
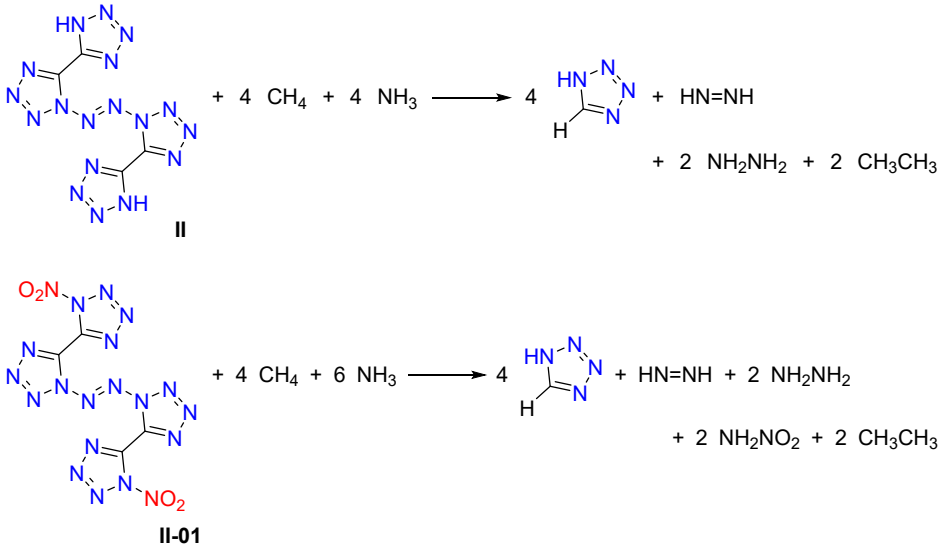
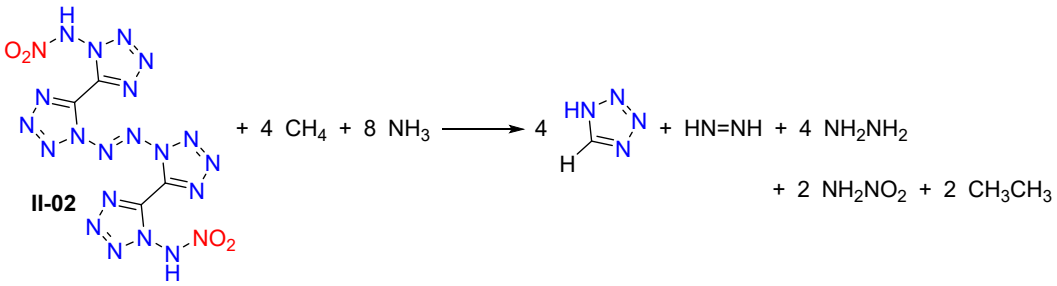
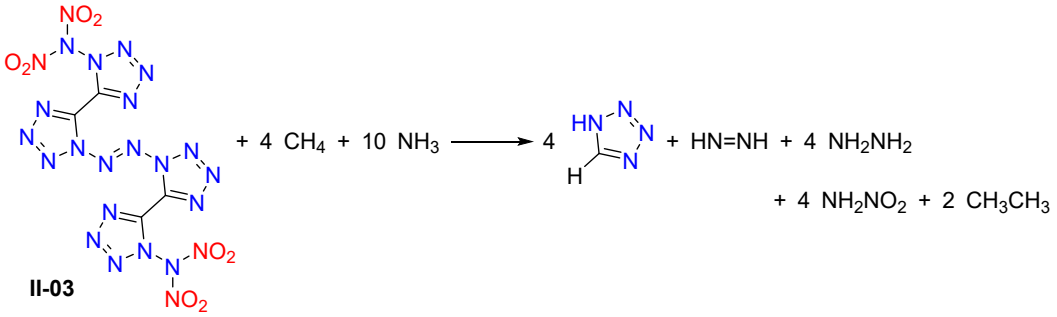
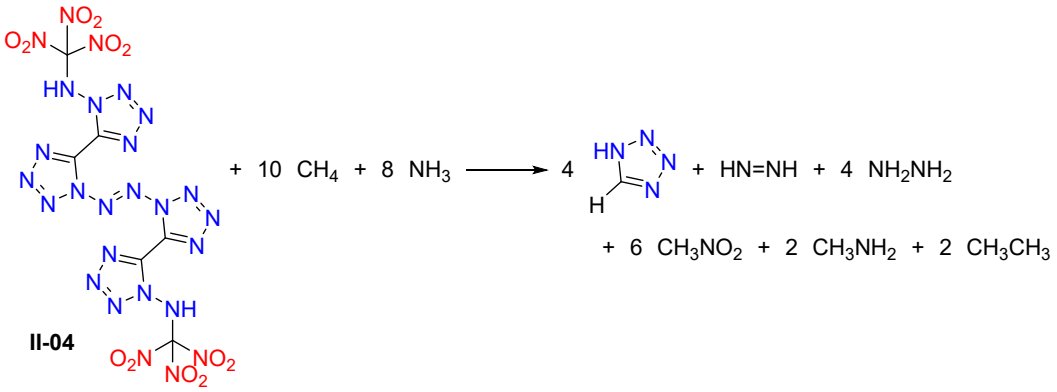


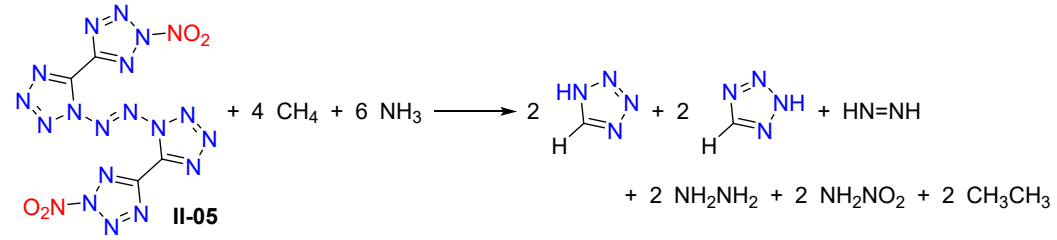
Fig. **S3** Isodesmic reactions of series **I** designed molecules

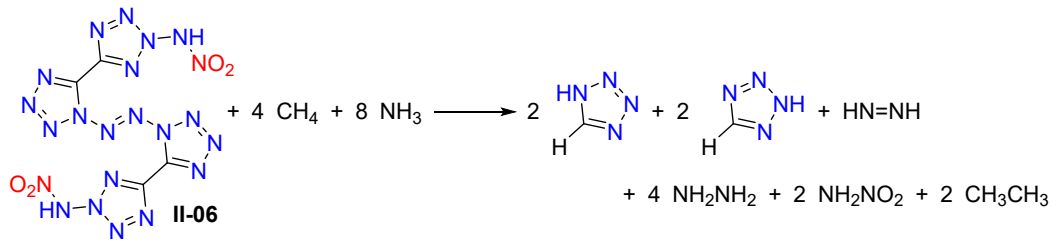


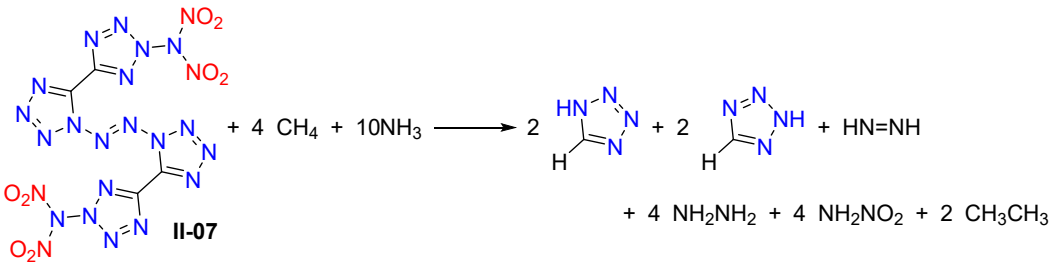

II-02
+ 4 CH4 + 8 NH3
4
+ HN=NH + 4 NH2NH2
+ 2 NH2NO2 + 2 CH3CH3


II-03
+ 4 CH4 + 10 NH3
4
+ HN=NH + 4 NH2NH2
+ 4 NH2NO2 + 2 CH3CH3


II-04
+ 10 CH4 + 8 NH3
4
+ HN=NH + 4 NH2NH2
+ 6 CH3NO2 + 2 CH3NH2 + 2 CH3CH3


II-05
+ 4 CH4 + 6 NH3
2
+ 2
+ HN=NH
+ 2 NH2NH2 + 2 NH2NO2 + 2 CH3CH3


II-06
+ 4 CH4 + 8 NH3
2
+ 2
+ HN=NH
+ 4 NH2NH2 + 2 NH2NO2 + 2 CH3CH3


II-07
+ 4 CH4 + 10NH3
2
+ 2
+ HN=NH
+ 4 NH2NH2 + 4 NH2NO2 + 2 CH3CH3

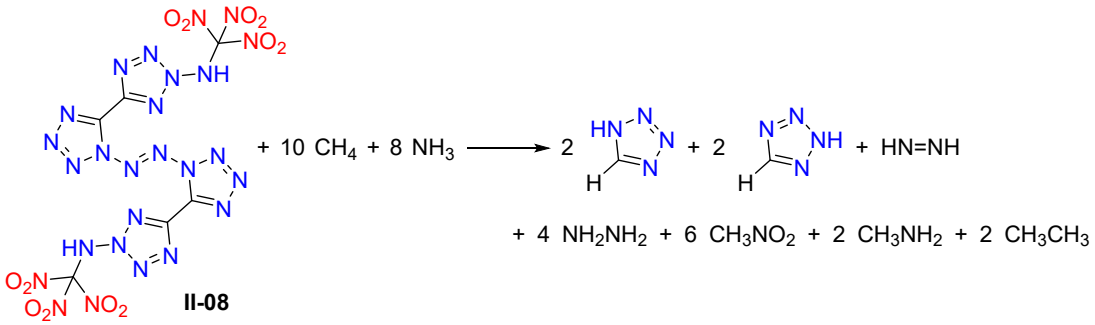
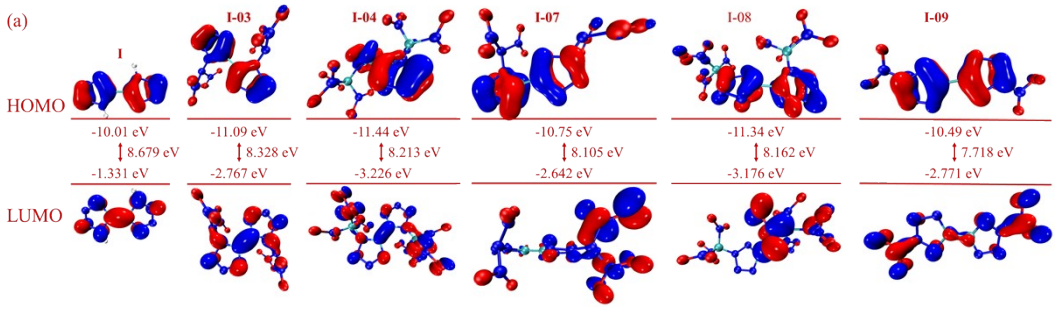


Fig. **S4** Isodesmic reactions of series **II** designed molecules

Table **S1** Density of designed molecules (at M06-2X/6-311g+(2d,p) level)

No.	Volume [a]	Density [b]	overall surface area [c]	$v\sigma_{tot}^2$ [d]	ρ [e]	ΔH_{vap} [f]	ΔH_{sub} [g]	T_{bp} [h]
I	141.3 (140.6) [i]	1.623 (1.631) [i]	150.3 (150.1) [i]	41.64 (44.09) [i]	1.651 (1.665) [i]	14.27 (14.42) [i]	82.12 (83.33) [i]	554.1 (559.7) [i]
I-01	201.9	1.876	202.9	18.13	1.818	16.46	87.72	625.0
I-02	234.1	1.831	225.8	18.81	1.778	18.20	99.21	690.2
I-03	290.7	**1.989**	267.5	11.78	1.904	20.18	115.9	774.0
I-04	357.9	**2.023**	314.3	5.98	1.919	22.19	139.5	869.4
I-05	202.3	1.872	207.4	25.53	1.835	17.53	95.26	663.7
I-06	235.5	1.820	233.4	45.31	1.842	20.96	119.6	790.7
I-07	294.3	**1.964**	280.8	30.32	1.933	22.97	138.4	879.6
I-08	363.3	**1.993**	320.1	11.73	1.908	23.45	150.4	917.8
I-09	203.1	1.865	210.7	18.65	1.809	17.09	91.73	648.3
I-10	237.8	1.803	242.6	27.36	1.776	20.20	114.2	766.0
I-11	298.0	**1.940**	293.7	13.38	1.863	22.06	133.9	853.4
I-12	365.6	**1.981**	341.1	6.66	1.882	23.89	160.0	947.1
II	288.8	1.738	280.3	50.13	1.780	24.40	148.9	930.7
II-01	349.7	1.862	334.8	23.66	1.821	25.65	171.0	1006
II-02	381.3	1.839	349.3	30.10	1.817	27.07	186.4	1066
II-03	442.1	**1.924**	400.8	23.19	1.876	29.28	224.92	1185
II-04	503.9	**1.978**	430.8	15.88	1.905	30.07	247.0	1239
II-05	351.9	1.851	345.7	27.99	1.822	26.68	182.3	1050
II-06	386.6	1.814	377.4	35.18	1.808	29.05	212.2	1158
II-07	446.6	**1.904**	428.2	29.68	1.876	31.30	254.6	1281
II-08	513.7	**1.940**	475.5	22.45	1.889	33.01	297.4	1387

[a] Angstrom^3; [b] Estimated density according to mass and volume, g/cm^3; [c] Angstrom^2; [d] Product of sigma^2_tot and nu, (kcal/mol)^2; [e] $\rho = \alpha\frac{M}{V_m} + \beta\left(v\sigma_{tot}^2\right) + \gamma$, $\alpha = 0.9183$, $\beta = 0.0028$, $\gamma = 0.0443$ (*ref*: *Mol. Phys.* 2009, **107**, 2095-2101.); [f] $\Delta H_{vap} = a\sqrt{A} + b\sqrt{v\sigma_{tot}^2} + c$ (kal/mol), $a = 2.130$, $b = 0.930$, $c = -17.844$ (*ref*: *J. Phys. Chem. A.* 2006, **110(3)**, 1005-1013.); [g] $\Delta H_{sub} = aA^2 + b\sqrt{v\sigma_{tot}^2} + c$ (kJ/mol), $a = 0.000267$, $b = 1.650087$, $c = 2.966078$; [h] $T_{bp} = \alpha A + \beta\sqrt{v\sigma_{tot}^2} + \gamma$ (K), $\alpha = 2.736$, $\beta = 33.31$, $\gamma = -72.05$ (*ref*: *J. Phys. Chem.* 1993, **97(37)**, 9369-9373.); [i] calculated at MP2/6-311g+(2d,p) level



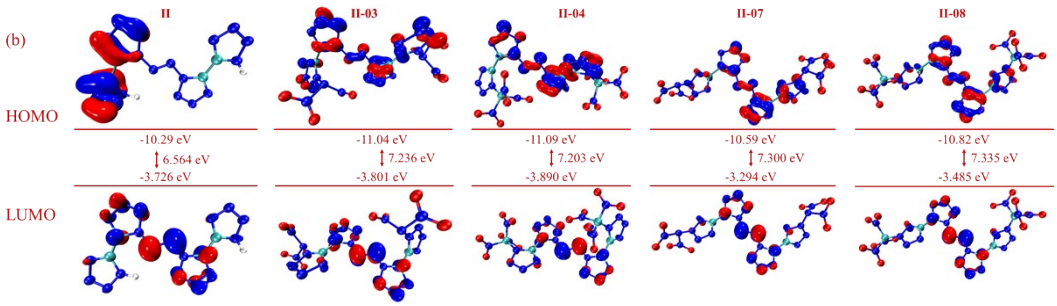


Fig. **S5** HOMO-LUMO energy gaps of series **I** and series **II** at M06-2X/6-311g+(2d,p) level

Based on the designed isodesmic reactions (Fig. **S3** and **S4**), the heat of formation (HOFs) for the designed molecules could be determined using the following formula:

$$\Delta H_f^0(gas,298\ K) = \sum \Delta H_{f,P}^0(gas,298\ K) - \sum \Delta H_{f,R}^0(gas,298\ K) = \Delta E_0 + \Delta E_{ZPE} + \Delta H_T + \Delta nRT$$

(eq. 1)

$$\Delta H_f^0(solid,298\ k) = \Delta H_f^0(gas,298\ K) - \Delta H_{sub} \quad \textbf{(eq. 2)}$$

Table **S2** HOFs of designed molecules (at M06-2X/6-311g+(2d,p) level)

No.	E_{ZPE} [a]	ΔH_T^0 [a]	E_0 [a]	$\Delta H_f^0(gas)$ [b]	$\Delta H_f^0(solid)$ [b]	h_{50} [c]
I	0.0761	0.0838	-515.2	707.4	625.3	25.50 (24.96) [d]
I-01	0.0791	0.0921	-924.1	791.4	703.7	20.63
I-02	0.1153	0.1300	-1035	984.0	884.8	10.80
I-03	0.1173	0.1371	-1444	1068	952.1	25.08
I-04	0.1466	0.1710	-1821	713.8	574.3	16.84
I-05	0.0795	0.0924	-924.1	748.0	652.7	28.99
I-06	0.1155	0.1301	-1035	848.8	729.2	25.61
I-07	0.1173	0.1372	-1444	1025	886.3	47.91
I-08	0.1465	0.1720	-1821	670.4	520.0	24.51
I-09	0.0797	0.0926	-924.1	704.6	612.9	25.16
I-10	0.1155	0.1303	-1035	897.2	783.1	17.56
I-11	0.1175	0.1374	-1444	981.2	847.3	28.72
I-12	0.1467	0.1724	-1821	627.0	467.0	12.23
II	0.1401	0.1567	-1139	1900	1751	28.72
II-01	0.1435	0.1653	-1548	1984	1813	24.74
II-02	0.1792	0.2028	-1658	2176	1990	20.67
II-03	0.1808	0.2098	-2067	2260	2035	26.78
II-04	0.2106	0.2446	-2444	2099	1852	23.49
II-05	0.1437	0.1656	-1548	1897	1715	33.16
II-06	0.1793	0.2031	-1658	2090	1877	27.39
II-07	0.1813	0.2104	-2067	2174	1919	42.14
II-08	0.2107	0.2414	-2444	1609	1311	30.64

[a] a.u.; [b] kJ/mol; [c] $h_{50} = \alpha\sigma_+^2 + \beta v + \gamma$ (cm), $\alpha = -0.0064$, $\beta = 241.42$, $\gamma = -3.43$, $v = \frac{\sigma_+^2\sigma_-^2}{(\sigma_+^2 + \sigma_-^2)^2}$ (*ref*: *J. Mol. Model.* 2010, **16**, 895-901); [d] calculated at MP2/6-311g+(2d,p) level

Table **S3** Detonation properties of designed molecules (at M06-2X/6-311g+(2d,p) level)

No.	ρ [a]	ΔH_f^0 [b]	OB% [c]	Q [d]	D [e]	P [f]	h_{50} [g]
I	1.623	625.3	34.76	4850	7.323	22.31	25.50
I-01	1.876	703.7	40.38	5760	8.792	35.14	20.63
I-02	1.831	884.8	43.39	6645	9.127	37.32	10.80

I-03	1.989	952.1	45.96	7250	10.02	47.15	25.08
I-04	2.023	574.3	22.01	6724	9.778	45.36	16.84
I-05	1.872	652.7	42.09	6306	9.045	37.14	28.99
I-06	1.820	729.2	43.39	6043	8.876	35.17	25.61
I-07	1.964	886.3	45.96	7061	9.864	45.40	47.91
I-08	1.993	520.0	22.01	6600	9.628	43.61	24.51
I-09	1.865	612.9	42.09	6132	8.959	36.36	25.16
I-10	1.803	783.1	43.39	6251	8.892	35.10	17.56
I-11	1.940	847.3	45.96	6949	9.737	43.93	28.72
I-12	1.981	467.0	22.01	6478	9.541	42.68	12.23
II	1.738	1751	47.65	5937	8.098	28.48	28.72
II-01	1.862	1813	48.96	6622	8.972	36.43	24.74
II-02	1.839	1990	49.26	6677	8.986	36.28	20.67
II-03	1.924	2035	49.98	7040	9.522	41.81	26.78
II-04	1.978	1852	33.00	6749	9.566	42.87	23.49
II-05	1.851	1715	48.96	6372	8.848	35.30	33.16
II-06	1.814	1877	49.26	6411	8.809	34.58	27.39
II-07	1.904	1919	49.98	6813	9.376	40.31	42.14
II-08	1.940	1311	33.00	5892	9.119	38.54	30.64
RDX	1.758 (1.80 [h])	96.34	21.62	6351	8.693	33.04	34.01
HMX	1.809 (1.91 [h])	74.90	21.62	6171	8.805	34.49	29.78

[a] density (g/cm^3); [b] solid phase heat of formation (kJ/mol); [c] oxygen balance; [d] explosion heat (J/g); [e] detonation velocity (km/s); [f] explosion pressure (GPa); [g] impact sensitivity (cm); [h] *ref*: *Propellants Explos. Pyrotech.*, 2014, **39(3)**, 383-389; *Combust. Explos. Shock Waves*, 2009, **45(1)**, 78-87.

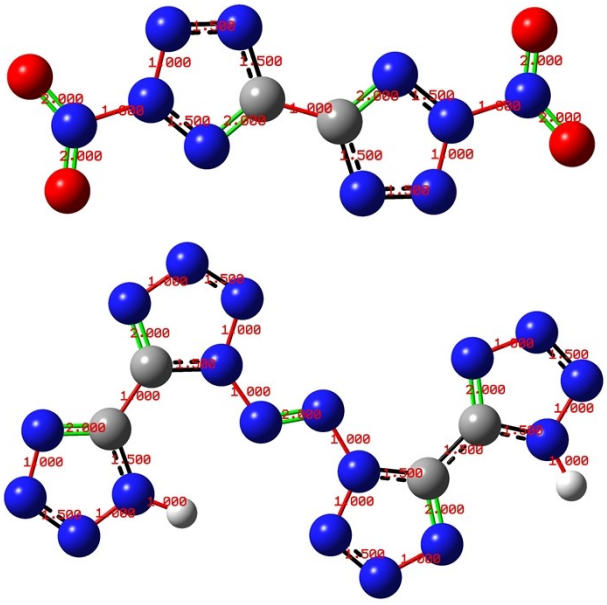


Fig. **S6** Bond order of molecule **I-09** and **II** (at M06-2X/6-311g+(2d,p) level)

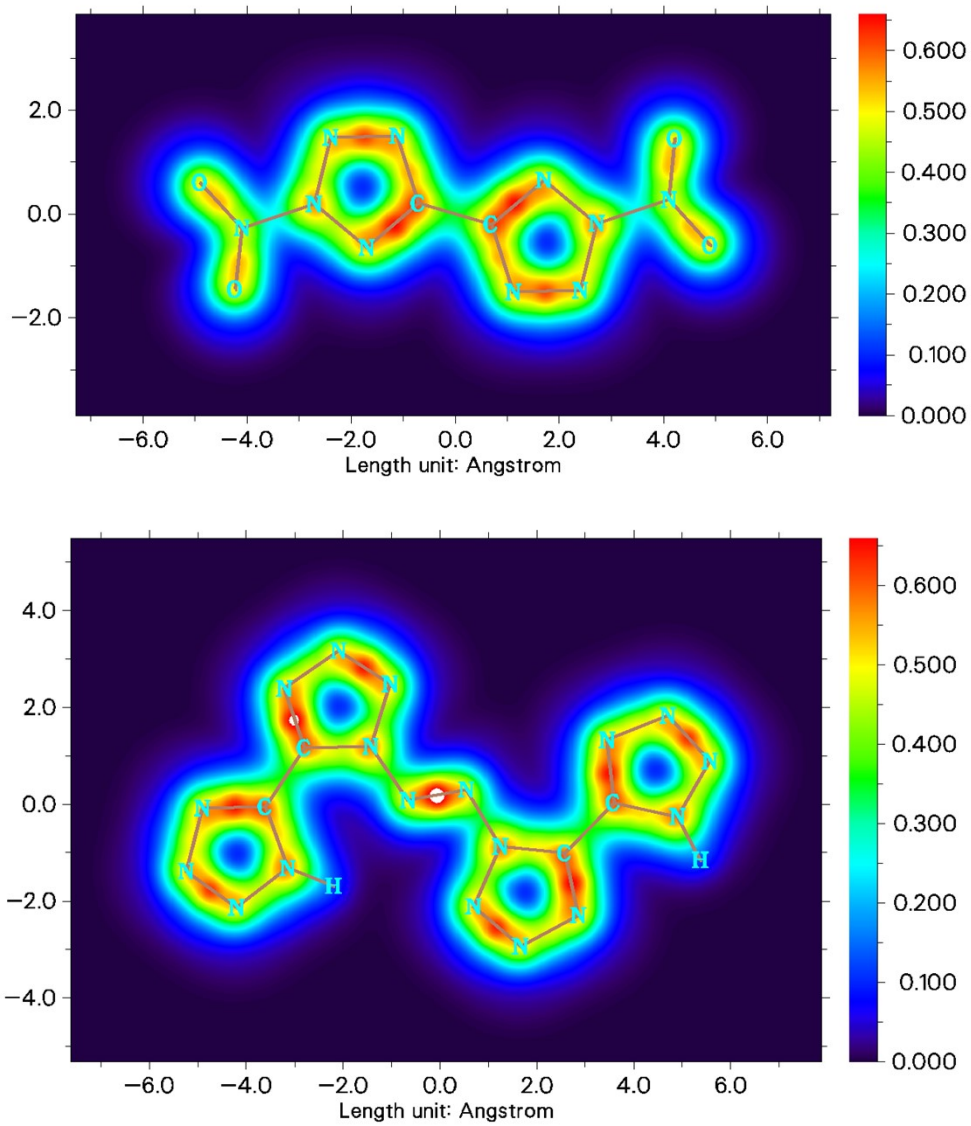


Fig. **S7** LOL-pi color filling map of molecule **I-09** and **II** (at M06-2X/6-311g+(2d,p) level)

Table **S4** The HOMA method was employed to assess the aromaticity of each ring within **I-09** and **II** (at M06-2X/6-311g+(2d,p) level)

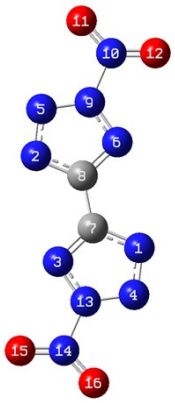
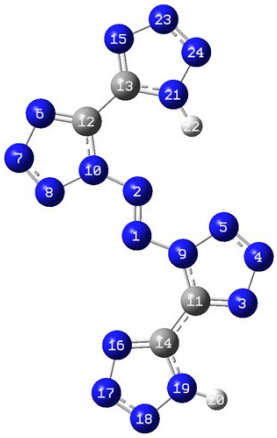
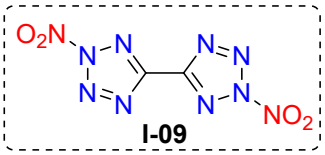
No.	Atom pair	Contribution	Bond length(Angstrom)
 **I-09**	1(N) -- 4(N)	-0.012506	1.287096
	4(N) -- 13(N)	-0.004631	1.322329
	13(N) -- 3(N)	-0.000107	1.311022
	3(N) -- 7(C)	-0.006149	1.315869
	7(C) -- 1(N)	-0.016834	1.364001
	HOMA value is 0.959774		
	2(N) -- 8(C)	-0.016859	1.364022
	8(C) -- 6(N)	-0.006161	1.315851
	6(N) -- 9(N)	-0.000107	1.311026
	9(N) -- 5(N)	-0.004649	1.322356
	5(N) -- 2(N)	-0.012538	1.287068
	HOMA value is 0.959686		
 **II**	13(C) -- 21(N)	-0.002726	1.346073
	21(N) -- 24(N)	-0.012638	1.331019
	24(N) -- 23(N)	-0.016444	1.283883
	23(N) -- 15(N)	-0.033864	1.345044
	15(N) -- 13(C)	-0.010161	1.310692
	HOMA value is 0.924168		
	12(C) -- 10(N)	-0.014015	1.361373
	10(N) -- 8(N)	-0.050263	1.352912
	8(N) -- 7(N)	-0.040576	1.269545
	7(N) -- 6(N)	-0.085024	1.366113
	6(N) -- 12(C)	-0.021428	1.300153
	HOMA value is 0.788694		
	9(N) -- 5(N)	-0.046091	1.351051
	5(N) -- 4(N)	-0.036027	1.271823
	4(N) -- 3(N)	-0.057520	1.355976
	3(N) -- 11(C)	-0.014139	1.306506
	11(C) -- 9(N)	-0.005376	1.350953
	HOMA value is 0.840847		
	14(C) -- 16(N)	-0.011807	1.308876
	16(N) -- 17(N)	-0.042106	1.349191
	17(N) -- 18(N)	-0.016784	1.283625
	18(N) -- 19(N)	-0.011438	1.329948
	19(N) -- 14(C)	-0.001070	1.341562
	HOMA value is 0.916796		

Table **S5** The FiPC-NICS index [a] for **I-09**, **II** and each ring within both **I-09** and **II** (at M06-2X/6-311g+(2d,p) level)

No.	FiPC-NICS.txt [b]
	The scanning direction is found to be Z
	FiPC-NICS is -2.048266 ppm, at 1.464 Angstrom1
	1 0.000 -8.681233 -11.443733
	2 0.050 -8.718067 -11.319400
	3 0.101 -8.819533 -10.956400
	4 0.151 -8.960267 -10.383200
	5 0.201 -9.104233 -9.642533
	6 0.251 -9.211633 -8.785567
	7 0.302 -9.246100 -7.865667
	8 0.352 -9.180433 -6.932633
	9 0.402 -8.999300 -6.028900
	10 0.452 -8.699967 -5.187100
	11 0.503 -8.290733 -4.429633
	12 0.553 -7.787900 -3.769133
	13 0.603 -7.212900 -3.210233
	14 0.653 -6.589067 -2.751167
	15 0.704 -5.939467 -2.385800
	16 0.754 -5.284900 -2.105233
	17 0.804 -4.643200 -1.899133
	18 0.854 -4.028433 -1.756667
	19 0.905 -3.451033 -1.667233
	20 0.955 -2.917967 -1.620933
	21 1.005 -2.433167 -1.608733
	22 1.055 -1.997900 -1.622600
	23 1.106 -1.611533 -1.655667
	24 1.156 -1.271933 -1.701967
	25 1.206 -0.975967 -1.756667
	26 1.256 -0.719833 -1.815767
	27 1.307 -0.499633 -1.876033
	28 1.357 -0.311267 -1.935000
	29 1.407 -0.151000 -1.990833
	30 1.457 -0.015200 -2.042167
	31 1.508 0.099267 -2.088100
	32 1.558 0.195333 -2.128067
	33 1.608 0.275367 -2.161833
	34 1.658 0.341633 -2.189267
	35 1.709 0.395967 -2.210500
	36 1.759 0.439933 -2.225733
	37 1.809 0.475033 -2.235267
	38 1.859 0.502300 -2.239467
	39 1.910 0.522933 -2.238700
	40 1.960 0.537733 -2.233400
	41 2.010 0.547567 -2.223967
	42 2.060 0.553167 -2.210767
	43 2.111 0.555100 -2.194233
	44 2.161 0.554000 -2.174733
	45 2.211 0.550333 -2.152600
	46 2.261 0.544567 -2.128167
	47 2.312 0.537033 -2.101767
	48 2.362 0.528200 -2.073600
	49 2.412 0.518233 -2.044033
	50 2.462 0.507533 -2.013200
	51 2.513 0.496200 -1.981367
	52 2.563 0.484533 -1.948733
	53 2.613 0.472633 -1.915467
	54 2.663 0.460633 -1.881733
	55 2.714 0.448633 -1.847633
	56 2.764 0.436767 -1.813333
	57 2.814 0.425033 -1.778933
	58 2.864 0.413600 -1.744567
	59 2.915 0.402367 -1.710233
	60 2.965 0.391467 -1.676100
	61 3.015 0.380867 -1.642200

I-09

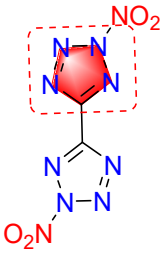
62	3.065	0.370600	-1.608600
63	3.116	0.360667	-1.575333
64	3.166	0.351067	-1.542467
65	3.216	0.341767	-1.510000
66	3.266	0.332833	-1.478033
67	3.317	0.324200	-1.446533
68	3.367	0.315900	-1.415567
69	3.417	0.307833	-1.385133
70	3.467	0.300100	-1.355233
71	3.518	0.292633	-1.325900
72	3.568	0.285433	-1.297133
73	3.618	0.278500	-1.268933
74	3.668	0.271800	-1.241333
75	3.719	0.265333	-1.214300
76	3.769	0.259067	-1.187833
77	3.819	0.253033	-1.161967
78	3.869	0.247200	-1.136667
79	3.920	0.241533	-1.111933
80	3.970	0.236100	-1.087767
81	4.020	0.230800	-1.064167
82	4.070	0.225667	-1.041133
83	4.121	0.220733	-1.018600
84	4.171	0.215900	-0.996633
85	4.221	0.211233	-0.975200
86	4.271	0.206733	-0.954267
87	4.322	0.202300	-0.933833
88	4.372	0.198067	-0.913900
89	4.422	0.193900	-0.894433
90	4.472	0.189867	-0.875467
91	4.523	0.185967	-0.856967
92	4.573	0.182167	-0.838933
93	4.623	0.178467	-0.821333
94	4.673	0.174867	-0.804133
95	4.724	0.171333	-0.787400
96	4.774	0.167933	-0.771067
97	4.824	0.164633	-0.755133
98	4.874	0.161400	-0.739600
99	4.925	0.158233	-0.724433
100	4.975	0.155167	-0.709667
101	5.025	0.152167	-0.695233
102	5.075	0.149233	-0.681167
103	5.126	0.146433	-0.667433
104	5.176	0.143633	-0.654067
105	5.226	0.140900	-0.641000
106	5.276	0.138300	-0.628267
107	5.327	0.135700	-0.615833
108	5.377	0.133200	-0.603700
109	5.427	0.130733	-0.591867
110	5.477	0.128333	-0.580333
111	5.528	0.126000	-0.569033
112	5.578	0.123733	-0.558033
113	5.628	0.121467	-0.547300
114	5.678	0.119300	-0.536833
115	5.729	0.117200	-0.526600
116	5.779	0.115100	-0.516600
117	5.829	0.113067	-0.506833
118	5.879	0.111067	-0.497300
119	5.930	0.109133	-0.488000
120	5.980	0.107233	-0.478900
121	6.030	0.105367	-0.470033
122	6.080	0.103567	-0.461367
123	6.131	0.101767	-0.452900
124	6.181	0.100033	-0.444633
125	6.231	0.098333	-0.436533
126	6.281	0.096667	-0.428633
127	6.332	0.095067	-0.420900
128	6.382	0.093433	-0.413367

129	6.432	0.091900	-0.405967
130	6.482	0.090367	-0.398767
131	6.533	0.088867	-0.391733
132	6.583	0.087400	-0.384833
133	6.633	0.085967	-0.378100
134	6.683	0.084567	-0.371500
135	6.734	0.083200	-0.365067
136	6.784	0.081833	-0.358733
137	6.834	0.080533	-0.352567
138	6.884	0.079267	-0.346533
139	6.935	0.077967	-0.340633
140	6.985	0.076733	-0.334867
141	7.035	0.075533	-0.329233
142	7.085	0.074367	-0.323700
143	7.136	0.073167	-0.318267
144	7.186	0.072033	-0.312967
145	7.236	0.070933	-0.307800
146	7.286	0.069800	-0.302733
147	7.337	0.068733	-0.297733
148	7.387	0.067667	-0.292900
149	7.437	0.066633	-0.288133
150	7.487	0.065633	-0.283467
151	7.538	0.064633	-0.278900
152	7.588	0.063633	-0.274400
153	7.638	0.062700	-0.270033
154	7.688	0.061767	-0.265733
155	7.739	0.060833	-0.261533
156	7.789	0.059933	-0.257400
157	7.839	0.059067	-0.253367
158	7.889	0.058167	-0.249400
159	7.940	0.057333	-0.245533
160	7.990	0.056500	-0.241733
161	8.040	0.055667	-0.238000
162	8.090	0.054867	-0.234333
163	8.141	0.054067	-0.230767
164	8.191	0.053267	-0.227233
165	8.241	0.052533	-0.223800
166	8.291	0.051767	-0.220433
167	8.342	0.051067	-0.217100
168	8.392	0.050300	-0.213867
169	8.442	0.049600	-0.210667
170	8.492	0.048933	-0.207567
171	8.543	0.048200	-0.204500
172	8.593	0.047533	-0.201467
173	8.643	0.046867	-0.198533
174	8.693	0.046233	-0.195633
175	8.744	0.045600	-0.192800
176	8.794	0.045000	-0.190000
177	8.844	0.044367	-0.187267
178	8.894	0.043733	-0.184600
179	8.945	0.043167	-0.181933
180	8.995	0.042567	-0.179367
181	9.045	0.042000	-0.176833
182	9.095	0.041467	-0.174333
183	9.146	0.040867	-0.171867
184	9.196	0.040333	-0.169467
185	9.246	0.039800	-0.167100
186	9.296	0.039267	-0.164800
187	9.347	0.038767	-0.162533
188	9.397	0.038267	-0.160267
189	9.447	0.037733	-0.158100
190	9.497	0.037233	-0.155933
191	9.548	0.036767	-0.153800
192	9.598	0.036300	-0.151733
193	9.648	0.035833	-0.149667
194	9.698	0.035367	-0.147667
195	9.749	0.034900	-0.145700

196	9.799	0.034467	-0.143733
197	9.849	0.034033	-0.141833
198	9.899	0.033600	-0.139967
199	9.950	0.033200	-0.138133
200	10.000	0.032733	-0.136300

The scanning direction is found to be Z
FiPC-NICS is -7.096105 ppm, at 1.506 Angstrom

1	0.000	-7.573000	-3.632467
2	0.050	-7.539833	-3.711900
3	0.101	-7.441233	-3.945367
4	0.151	-7.279633	-4.319333
5	0.201	-7.059100	-4.812633
6	0.251	-6.785200	-5.398367
7	0.302	-6.464700	-6.046067
8	0.352	-6.105600	-6.724200
9	0.402	-5.716667	-7.402233
10	0.452	-5.306867	-8.052633
11	0.503	-4.885300	-8.652000
12	0.553	-4.460433	-9.182100
13	0.603	-4.040000	-9.630000
14	0.653	-3.630600	-9.988067
15	0.704	-3.237667	-10.253367
16	0.754	-2.865367	-10.427033
17	0.804	-2.516500	-10.513433
18	0.854	-2.192867	-10.519300
19	0.905	-1.895233	-10.452933
20	0.955	-1.623600	-10.323600
21	1.005	-1.377333	-10.140833
22	1.055	-1.155333	-9.913967
23	1.106	-0.956267	-9.651867
24	1.156	-0.778533	-9.362767
25	1.206	-0.620533	-9.053967
26	1.256	-0.480600	-8.731867
27	1.307	-0.357033	-8.402033
28	1.357	-0.248433	-8.069100
29	1.407	-0.153267	-7.736900
30	1.457	-0.070133	-7.408567
31	1.508	0.002133	-7.086600
32	1.558	0.064733	-6.772867
33	1.608	0.118767	-6.468800
34	1.658	0.165100	-6.175467
35	1.709	0.204633	-5.893533
36	1.759	0.238167	-5.623400
37	1.809	0.266400	-5.365300
38	1.859	0.290000	-5.119200
39	1.910	0.309467	-4.885000
40	1.960	0.325367	-4.662467
41	2.010	0.338167	-4.451300
42	2.060	0.348200	-4.251100
43	2.111	0.355933	-4.061433
44	2.161	0.361600	-3.881900
45	2.211	0.365467	-3.712000
46	2.261	0.367867	-3.551300
47	2.312	0.368933	-3.399333
48	2.362	0.368900	-3.255633
49	2.412	0.367867	-3.119733
50	2.462	0.366067	-2.991200
51	2.513	0.363567	-2.869667
52	2.563	0.360500	-2.754667
53	2.613	0.356900	-2.645833
54	2.663	0.352900	-2.542800
55	2.714	0.348600	-2.445233
56	2.764	0.343967	-2.352833
57	2.814	0.339133	-2.265200
58	2.864	0.334100	-2.182133
59	2.915	0.328933	-2.103300
60	2.965	0.323633	-2.028467



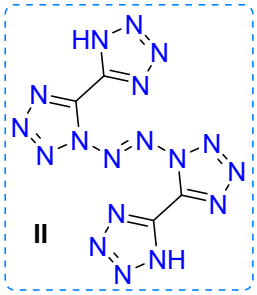
61	3.015	0.318233	-1.957367
62	3.065	0.312800	-1.889833
63	3.116	0.307367	-1.825567
64	3.166	0.301900	-1.764433
65	3.216	0.296400	-1.706200
66	3.266	0.290933	-1.650733
67	3.317	0.285500	-1.597867
68	3.367	0.280133	-1.547433
69	3.417	0.274767	-1.499267
70	3.467	0.269500	-1.453267
71	3.518	0.264300	-1.409300
72	3.568	0.259133	-1.367267
73	3.618	0.254067	-1.327000
74	3.668	0.249067	-1.288467
75	3.719	0.244133	-1.251567
76	3.769	0.239333	-1.216167
77	3.819	0.234567	-1.182200
78	3.869	0.229900	-1.149600
79	3.920	0.225367	-1.118300
80	3.970	0.220867	-1.088200
81	4.020	0.216467	-1.059267
82	4.070	0.212167	-1.031433
83	4.121	0.207933	-1.004667
84	4.171	0.203833	-0.978867
85	4.221	0.199800	-0.954000
86	4.271	0.195833	-0.930033
87	4.322	0.191933	-0.906933
88	4.372	0.188133	-0.884633
89	4.422	0.184433	-0.863100
90	4.472	0.180833	-0.842300
91	4.523	0.177267	-0.822233
92	4.573	0.173800	-0.802800
93	4.623	0.170400	-0.784033
94	4.673	0.167100	-0.765867
95	4.724	0.163833	-0.748300
96	4.774	0.160700	-0.731300
97	4.824	0.157600	-0.714800
98	4.874	0.154567	-0.698833
99	4.925	0.151600	-0.683367
100	4.975	0.148733	-0.668367
101	5.025	0.145900	-0.653800
102	5.075	0.143133	-0.639700
103	5.126	0.140433	-0.626000
104	5.176	0.137767	-0.612700
105	5.226	0.135233	-0.599800
106	5.276	0.132667	-0.587267
107	5.327	0.130233	-0.575100
108	5.377	0.127833	-0.563233
109	5.427	0.125467	-0.551733
110	5.477	0.123167	-0.540567
111	5.528	0.120933	-0.529667
112	5.578	0.118700	-0.519100
113	5.628	0.116567	-0.508800
114	5.678	0.114467	-0.498767
115	5.729	0.112433	-0.489000
116	5.779	0.110400	-0.479500
117	5.829	0.108467	-0.470233
118	5.879	0.106567	-0.461233
119	5.930	0.104633	-0.452433
120	5.980	0.102800	-0.443900
121	6.030	0.101033	-0.435533
122	6.080	0.099267	-0.427400
123	6.131	0.097567	-0.419467
124	6.181	0.095867	-0.411733
125	6.231	0.094233	-0.404200
126	6.281	0.092667	-0.396833
127	6.332	0.091067	-0.389667

128	6.382	0.089533	-0.382633
129	6.432	0.088033	-0.375800
130	6.482	0.086567	-0.369100
131	6.533	0.085133	-0.362600
132	6.583	0.083700	-0.356233
133	6.633	0.082333	-0.350000
134	6.683	0.081000	-0.343900
135	6.734	0.079633	-0.337967
136	6.784	0.078367	-0.332167
137	6.834	0.077100	-0.326500
138	6.884	0.075833	-0.320933
139	6.935	0.074633	-0.315533
140	6.985	0.073433	-0.310233
141	7.035	0.072267	-0.305033
142	7.085	0.071133	-0.299967
143	7.136	0.070000	-0.295000
144	7.186	0.068933	-0.290133
145	7.236	0.067833	-0.285400
146	7.286	0.066767	-0.280767
147	7.337	0.065733	-0.276200
148	7.387	0.064733	-0.271767
149	7.437	0.063767	-0.267400
150	7.487	0.062767	-0.263133
151	7.538	0.061800	-0.258967
152	7.588	0.060867	-0.254867
153	7.638	0.059967	-0.250867
154	7.688	0.059067	-0.246933
155	7.739	0.058200	-0.243100
156	7.789	0.057300	-0.239333
157	7.839	0.056467	-0.235633
158	7.889	0.055667	-0.232033
159	7.940	0.054800	-0.228500
160	7.990	0.054000	-0.225000
161	8.040	0.053233	-0.221600
162	8.090	0.052467	-0.218267
163	8.141	0.051733	-0.215000
164	8.191	0.050967	-0.211800
165	8.241	0.050233	-0.208667
166	8.291	0.049533	-0.205567
167	8.342	0.048833	-0.202567
168	8.392	0.048133	-0.199600
169	8.442	0.047467	-0.196667
170	8.492	0.046800	-0.193833
171	8.543	0.046133	-0.191033
172	8.593	0.045500	-0.188267
173	8.643	0.044867	-0.185567
174	8.693	0.044233	-0.182933
175	8.744	0.043667	-0.180333
176	8.794	0.043033	-0.177800
177	8.844	0.042467	-0.175300
178	8.894	0.041867	-0.172833
179	8.945	0.041333	-0.170433
180	8.995	0.040733	-0.168067
181	9.045	0.040200	-0.165733
182	9.095	0.039667	-0.163433
183	9.146	0.039167	-0.161200
184	9.196	0.038633	-0.159000
185	9.246	0.038133	-0.156833
186	9.296	0.037600	-0.154700
187	9.347	0.037100	-0.152633
188	9.397	0.036667	-0.150567
189	9.447	0.036167	-0.148567
190	9.497	0.035733	-0.146567
191	9.548	0.035233	-0.144633
192	9.598	0.034800	-0.142733
193	9.648	0.034333	-0.140833
194	9.698	0.033900	-0.139000

195	9.749	0.033500 -0.137200
196	9.799	0.033033 -0.135400
197	9.849	0.032633 -0.133633
198	9.899	0.032233 -0.131933
199	9.950	0.031833 -0.130233
200	10.000	0.031433 -0.128567

The scanning direction is found to be Z
FiPC-NICS is -1.305290 ppm, at 1.605 Angstrom

1	0.000	-21.329300	-15.132900
2	0.050	-21.602833	-15.001400
3	0.101	-22.352267	-14.619467
4	0.151	-23.392367	-14.019867
5	0.201	-24.473200	-13.250400
6	0.251	-25.344133	-12.365900
7	0.302	-25.807300	-11.420233
8	0.352	-25.748333	-10.460267
9	0.402	-25.140367	-9.522533
10	0.452	-24.029000	-8.632167
11	0.503	-22.507533	-7.804133
12	0.553	-20.691833	-7.045267
13	0.603	-18.700167	-6.356667
14	0.653	-16.639600	-5.735767
15	0.704	-14.598833	-5.178200
16	0.754	-12.645633	-4.678800
17	0.804	-10.827167	-4.232333
18	0.854	-9.172267	-3.833867
19	0.905	-7.694533	-3.478833
20	0.955	-6.395700	-3.163100
21	1.005	-5.269067	-2.883000
22	1.055	-4.302233	-2.635067
23	1.106	-3.479733	-2.416267
24	1.156	-2.784833	-2.223733
25	1.206	-2.200967	-2.054867
26	1.256	-1.712633	-1.907200
27	1.307	-1.305767	-1.778533
28	1.357	-0.967933	-1.666800
29	1.407	-0.688433	-1.570133
30	1.457	-0.458233	-1.486800
31	1.508	-0.269467	-1.415200
32	1.558	-0.115667	-1.353900
33	1.608	0.008700	-1.301633
34	1.658	0.108333	-1.257167
35	1.709	0.187267	-1.219500
36	1.759	0.248900	-1.187667
37	1.809	0.296167	-1.160867
38	1.859	0.331500	-1.138267
39	1.910	0.357167	-1.119300
40	1.960	0.374967	-1.103367
41	2.010	0.386400	-1.089967
42	2.060	0.392833	-1.078600
43	2.111	0.395433	-1.069000
44	2.161	0.395033	-1.060733
45	2.211	0.392433	-1.053567
46	2.261	0.388200	-1.047267
47	2.312	0.382900	-1.041633
48	2.362	0.376833	-1.036433
49	2.412	0.370300	-1.031600
50	2.462	0.363600	-1.027000
51	2.513	0.356800	-1.022467
52	2.563	0.350033	-1.018000
53	2.613	0.343433	-1.013500
54	2.663	0.337000	-1.008933
55	2.714	0.330733	-1.004200
56	2.764	0.324700	-0.999333
57	2.814	0.318900	-0.994267
58	2.864	0.313333	-0.989033
59	2.915	0.307900	-0.983567



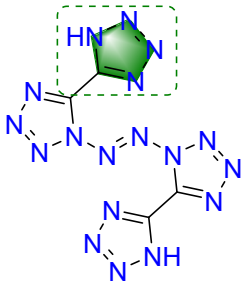
II

60	2.965	0.302700	-0.977867
61	3.015	0.297700	-0.971967
62	3.065	0.292833	-0.965833
63	3.116	0.288133	-0.959467
64	3.166	0.283533	-0.952933
65	3.216	0.279133	-0.946167
66	3.266	0.274767	-0.939200
67	3.317	0.270533	-0.932033
68	3.367	0.266433	-0.924700
69	3.417	0.262433	-0.917200
70	3.467	0.258467	-0.909533
71	3.518	0.254600	-0.901700
72	3.568	0.250800	-0.893767
73	3.618	0.247133	-0.885667
74	3.668	0.243467	-0.877500
75	3.719	0.239867	-0.869200
76	3.769	0.236367	-0.860800
77	3.819	0.232900	-0.852333
78	3.869	0.229533	-0.843800
79	3.920	0.226200	-0.835167
80	3.970	0.222867	-0.826500
81	4.020	0.219633	-0.817800
82	4.070	0.216433	-0.809067
83	4.121	0.213333	-0.800300
84	4.171	0.210233	-0.791500
85	4.221	0.207167	-0.782700
86	4.271	0.204167	-0.773900
87	4.322	0.201200	-0.765100
88	4.372	0.198300	-0.756300
89	4.422	0.195433	-0.747500
90	4.472	0.192633	-0.738767
91	4.523	0.189833	-0.730033
92	4.573	0.187100	-0.721300
93	4.623	0.184367	-0.712633
94	4.673	0.181733	-0.704033
95	4.724	0.179100	-0.695433
96	4.774	0.176500	-0.686900
97	4.824	0.173967	-0.678433
98	4.874	0.171467	-0.670000
99	4.925	0.168967	-0.661633
100	4.975	0.166567	-0.653333
101	5.025	0.164133	-0.645067
102	5.075	0.161800	-0.636900
103	5.126	0.159433	-0.628800
104	5.176	0.157167	-0.620767
105	5.226	0.154900	-0.612800
106	5.276	0.152667	-0.604933
107	5.327	0.150467	-0.597100
108	5.377	0.148333	-0.589367
109	5.427	0.146200	-0.581733
110	5.477	0.144067	-0.574167
111	5.528	0.142033	-0.566667
112	5.578	0.140000	-0.559267
113	5.628	0.138000	-0.551933
114	5.678	0.136033	-0.544667
115	5.729	0.134100	-0.537533
116	5.779	0.132200	-0.530433
117	5.829	0.130300	-0.523467
118	5.879	0.128467	-0.516533
119	5.930	0.126633	-0.509700
120	5.980	0.124833	-0.502967
121	6.030	0.123067	-0.496333
122	6.080	0.121367	-0.489733
123	6.131	0.119633	-0.483267
124	6.181	0.117967	-0.476833
125	6.231	0.116267	-0.470533
126	6.281	0.114667	-0.464300

127	6.332	0.113033	-0.458133
128	6.382	0.111500	-0.452067
129	6.432	0.109900	-0.446067
130	6.482	0.108367	-0.440133
131	6.533	0.106867	-0.434300
132	6.583	0.105367	-0.428567
133	6.633	0.103933	-0.422900
134	6.683	0.102500	-0.417300
135	6.734	0.101100	-0.411767
136	6.784	0.099667	-0.406333
137	6.834	0.098333	-0.400967
138	6.884	0.096967	-0.395700
139	6.935	0.095633	-0.390467
140	6.985	0.094333	-0.385333
141	7.035	0.093067	-0.380267
142	7.085	0.091800	-0.375267
143	7.136	0.090567	-0.370333
144	7.186	0.089333	-0.365500
145	7.236	0.088100	-0.360700
146	7.286	0.086933	-0.356000
147	7.337	0.085767	-0.351367
148	7.387	0.084600	-0.346767
149	7.437	0.083467	-0.342267
150	7.487	0.082367	-0.337833
151	7.538	0.081267	-0.333433
152	7.588	0.080167	-0.329133
153	7.638	0.079133	-0.324867
154	7.688	0.078100	-0.320667
155	7.739	0.077033	-0.316533
156	7.789	0.076033	-0.312467
157	7.839	0.075033	-0.308467
158	7.889	0.074033	-0.304533
159	7.940	0.073067	-0.300633
160	7.990	0.072133	-0.296800
161	8.040	0.071200	-0.293000
162	8.090	0.070267	-0.289300
163	8.141	0.069367	-0.285633
164	8.191	0.068467	-0.282000
165	8.241	0.067600	-0.278433
166	8.291	0.066733	-0.274933
167	8.342	0.065867	-0.271467
168	8.392	0.065000	-0.268067
169	8.442	0.064200	-0.264733
170	8.492	0.063367	-0.261400
171	8.543	0.062600	-0.258167
172	8.593	0.061800	-0.254933
173	8.643	0.061000	-0.251800
174	8.693	0.060233	-0.248667
175	8.744	0.059500	-0.245600
176	8.794	0.058767	-0.242567
177	8.844	0.058033	-0.239600
178	8.894	0.057300	-0.236667
179	8.945	0.056600	-0.233767
180	8.995	0.055900	-0.230900
181	9.045	0.055233	-0.228100
182	9.095	0.054533	-0.225333
183	9.146	0.053867	-0.222600
184	9.196	0.053200	-0.219900
185	9.246	0.052567	-0.217267
186	9.296	0.051900	-0.214633
187	9.347	0.051300	-0.212067
188	9.397	0.050667	-0.209533
189	9.447	0.050067	-0.207033
190	9.497	0.049467	-0.204567
191	9.548	0.048867	-0.202133
192	9.598	0.048267	-0.199733
193	9.648	0.047700	-0.197400

194	9.698	0.047133 -0.195067
195	9.749	0.046567 -0.192767
196	9.799	0.046033 -0.190500
197	9.849	0.045467 -0.188300
198	9.899	0.044933 -0.186100
199	9.950	0.044433 -0.183933
200	10.000	0.043900 -0.181800

The scanning direction is found to be Z
FiPC-NICS is -8.953969 ppm, at 1.340 Angstrom



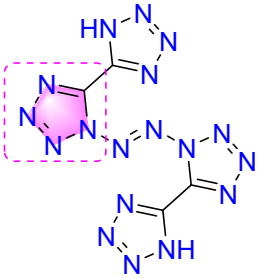
1	0.000	-6.068333	-4.906000
2	0.050	-6.042200	-4.987267
3	0.101	-5.964267	-5.226200
4	0.151	-5.836100	-5.608733
5	0.201	-5.660200	-6.112767
6	0.251	-5.440200	-6.710333
7	0.302	-5.181000	-7.369733
8	0.352	-4.888333	-8.058133
9	0.402	-4.568900	-8.743900
10	0.452	-4.229867	-9.398333
11	0.503	-3.878767	-9.997367
12	0.553	-3.522833	-10.522133
13	0.603	-3.168867	-10.959433
14	0.653	-2.822900	-11.301500
15	0.704	-2.489800	-11.545633
16	0.754	-2.173633	-11.693200
17	0.804	-1.877067	-11.749000
18	0.854	-1.601967	-11.720300
19	0.905	-1.349167	-11.616033
20	0.955	-1.118833	-11.446000
21	1.005	-0.910467	-11.220333
22	1.055	-0.723267	-10.948933
23	1.106	-0.556000	-10.641233
24	1.156	-0.407333	-10.305900
25	1.206	-0.275933	-9.950667
26	1.256	-0.160300	-9.582333
27	1.307	-0.059033	-9.206733
28	1.357	0.029233	-8.828800
29	1.407	0.105733	-8.452633
30	1.457	0.171633	-8.081467
31	1.508	0.228100	-7.718000
32	1.558	0.276067	-7.364167
33	1.608	0.316533	-7.021533
34	1.658	0.350267	-6.691133
35	1.709	0.378067	-6.373767
36	1.759	0.400667	-6.069800
37	1.809	0.418633	-5.779467
38	1.859	0.432567	-5.502767
39	1.910	0.442900	-5.239500
40	1.960	0.450233	-4.989500
41	2.010	0.454867	-4.752333
42	2.060	0.457233	-4.527600
43	2.111	0.457600	-4.314867
44	2.161	0.456267	-4.113633
45	2.211	0.453467	-3.923367
46	2.261	0.449500	-3.743533
47	2.312	0.444500	-3.573667
48	2.362	0.438700	-3.413200
49	2.412	0.432167	-3.261667
50	2.462	0.425100	-3.118533
51	2.513	0.417600	-2.983400
52	2.563	0.409733	-2.855733
53	2.613	0.401667	-2.735133
54	2.663	0.393433	-2.621167
55	2.714	0.385033	-2.513500
56	2.764	0.376600	-2.411667
57	2.814	0.368200	-2.315367
58	2.864	0.359800	-2.224267

59	2.915	0.351500	-2.138067
60	2.965	0.343267	-2.056400
61	3.015	0.335167	-1.979067
62	3.065	0.327200	-1.905733
63	3.116	0.319367	-1.836233
64	3.166	0.311700	-1.770267
65	3.216	0.304200	-1.707667
66	3.266	0.296933	-1.648200
67	3.317	0.289800	-1.591667
68	3.367	0.282867	-1.537933
69	3.417	0.276100	-1.486800
70	3.467	0.269567	-1.438133
71	3.518	0.263200	-1.391800
72	3.568	0.257000	-1.347600
73	3.618	0.251000	-1.305500
74	3.668	0.245200	-1.265300
75	3.719	0.239500	-1.226933
76	3.769	0.234033	-1.190267
77	3.819	0.228700	-1.155233
78	3.869	0.223533	-1.121733
79	3.920	0.218567	-1.089667
80	3.970	0.213700	-1.058967
81	4.020	0.208967	-1.029567
82	4.070	0.204400	-1.001367
83	4.121	0.199967	-0.974367
84	4.171	0.195667	-0.948433
85	4.221	0.191500	-0.923533
86	4.271	0.187433	-0.899600
87	4.322	0.183500	-0.876633
88	4.372	0.179700	-0.854533
89	4.422	0.175967	-0.833267
90	4.472	0.172367	-0.812833
91	4.523	0.168867	-0.793133
92	4.573	0.165467	-0.774133
93	4.623	0.162133	-0.755867
94	4.673	0.158933	-0.738200
95	4.724	0.155767	-0.721200
96	4.774	0.152767	-0.704767
97	4.824	0.149767	-0.688900
98	4.874	0.146900	-0.673600
99	4.925	0.144100	-0.658800
100	4.975	0.141367	-0.644500
101	5.025	0.138700	-0.630633
102	5.075	0.136100	-0.617233
103	5.126	0.133600	-0.604300
104	5.176	0.131100	-0.591733
105	5.226	0.128733	-0.579567
106	5.276	0.126400	-0.567800
107	5.327	0.124100	-0.556367
108	5.377	0.121900	-0.545300
109	5.427	0.119733	-0.534533
110	5.477	0.117633	-0.524133
111	5.528	0.115600	-0.514000
112	5.578	0.113567	-0.504167
113	5.628	0.111633	-0.494633
114	5.678	0.109733	-0.485367
115	5.729	0.107867	-0.476333
116	5.779	0.106033	-0.467567
117	5.829	0.104267	-0.459033
118	5.879	0.102533	-0.450767
119	5.930	0.100867	-0.442700
120	5.980	0.099200	-0.434833
121	6.030	0.097567	-0.427167
122	6.080	0.096000	-0.419733
123	6.131	0.094467	-0.412467
124	6.181	0.092967	-0.405400
125	6.231	0.091500	-0.398500

126	6.281	0.090033	-0.391800
127	6.332	0.088633	-0.385233
128	6.382	0.087267	-0.378867
129	6.432	0.085900	-0.372633
130	6.482	0.084600	-0.366533
131	6.533	0.083300	-0.360600
132	6.583	0.082067	-0.354800
133	6.633	0.080800	-0.349133
134	6.683	0.079600	-0.343600
135	6.734	0.078400	-0.338200
136	6.784	0.077267	-0.332933
137	6.834	0.076133	-0.327767
138	6.884	0.075033	-0.322733
139	6.935	0.073933	-0.317800
140	6.985	0.072867	-0.312967
141	7.035	0.071833	-0.308267
142	7.085	0.070800	-0.303633
143	7.136	0.069800	-0.299133
144	7.186	0.068800	-0.294733
145	7.236	0.067867	-0.290400
146	7.286	0.066933	-0.286167
147	7.337	0.065967	-0.282033
148	7.387	0.065100	-0.277967
149	7.437	0.064200	-0.274000
150	7.487	0.063300	-0.270100
151	7.538	0.062467	-0.266267
152	7.588	0.061633	-0.262533
153	7.638	0.060800	-0.258867
154	7.688	0.060000	-0.255267
155	7.739	0.059167	-0.251767
156	7.789	0.058400	-0.248300
157	7.839	0.057633	-0.244933
158	7.889	0.056867	-0.241600
159	7.940	0.056133	-0.238333
160	7.990	0.055400	-0.235167
161	8.040	0.054700	-0.232033
162	8.090	0.053967	-0.228933
163	8.141	0.053300	-0.225933
164	8.191	0.052633	-0.222967
165	8.241	0.051967	-0.220067
166	8.291	0.051300	-0.217200
167	8.342	0.050667	-0.214400
168	8.392	0.050033	-0.211633
169	8.442	0.049433	-0.208933
170	8.492	0.048800	-0.206267
171	8.543	0.048200	-0.203667
172	8.593	0.047600	-0.201100
173	8.643	0.047033	-0.198600
174	8.693	0.046467	-0.196100
175	8.744	0.045900	-0.193667
176	8.794	0.045333	-0.191300
177	8.844	0.044800	-0.188933
178	8.894	0.044267	-0.186633
179	8.945	0.043767	-0.184367
180	8.995	0.043233	-0.182133
181	9.045	0.042733	-0.179933
182	9.095	0.042233	-0.177767
183	9.146	0.041733	-0.175633
184	9.196	0.041233	-0.173533
185	9.246	0.040733	-0.171500
186	9.296	0.040300	-0.169467
187	9.347	0.039833	-0.167467
188	9.397	0.039367	-0.165500
189	9.447	0.038900	-0.163600
190	9.497	0.038467	-0.161700
191	9.548	0.038067	-0.159833
192	9.598	0.037633	-0.158000

193	9.648	0.037167	-0.156167
194	9.698	0.036767	-0.154400
195	9.749	0.036367	-0.152633
196	9.799	0.035967	-0.150900
197	9.849	0.035567	-0.149200
198	9.899	0.035200	-0.147533
199	9.950	0.034800	-0.145900
200	10.000	0.034400	-0.144267

The scanning direction is found to be Z
FiPC-NICS is -6.362663 ppm, at 1.455 Angstrom



1	0.000	-6.307167	-0.115500
2	0.050	-6.284233	-0.197233
3	0.101	-6.215700	-0.438067
4	0.151	-6.102100	-0.825567
5	0.201	-5.944667	-1.339900
6	0.251	-5.745400	-1.955900
7	0.302	-5.507333	-2.644800
8	0.352	-5.234467	-3.376367
9	0.402	-4.931900	-4.120933
10	0.452	-4.605767	-4.851167
11	0.503	-4.262700	-5.543200
12	0.553	-3.909667	-6.177767
13	0.603	-3.553500	-6.740267
14	0.653	-3.200600	-7.221000
15	0.704	-2.856633	-7.614867
16	0.754	-2.526367	-7.920633
17	0.804	-2.213500	-8.140467
18	0.854	-1.920700	-8.279033
19	0.905	-1.649633	-8.342900
20	0.955	-1.401200	-8.339900
21	1.005	-1.175433	-8.278367
22	1.055	-0.971900	-8.166867
23	1.106	-0.789733	-8.013800
24	1.156	-0.627700	-7.827067
25	1.206	-0.484433	-7.613867
26	1.256	-0.358433	-7.380733
27	1.307	-0.248167	-7.133400
28	1.357	-0.152133	-6.876833
29	1.407	-0.068900	-6.615200
30	1.457	0.002900	-6.352033
31	1.508	0.064600	-6.090133
32	1.558	0.117333	-5.831867
33	1.608	0.162200	-5.579000
34	1.658	0.200167	-5.332967
35	1.709	0.232100	-5.094733
36	1.759	0.258833	-4.865133
37	1.809	0.281000	-4.644567
38	1.859	0.299233	-4.433400
39	1.910	0.314067	-4.231667
40	1.960	0.325967	-4.039433
41	2.010	0.335333	-3.856567
42	2.060	0.342467	-3.682867
43	2.111	0.347733	-3.518100
44	2.161	0.351400	-3.361967
45	2.211	0.353633	-3.214133
46	2.261	0.354667	-3.074267
47	2.312	0.354667	-2.942000
48	2.362	0.353767	-2.817000
49	2.412	0.352100	-2.698833
50	2.462	0.349767	-2.587200
51	2.513	0.346867	-2.481733
52	2.563	0.343500	-2.382067
53	2.613	0.339667	-2.287900
54	2.663	0.335600	-2.198900
55	2.714	0.331167	-2.114767
56	2.764	0.326533	-2.035200
57	2.814	0.321733	-1.959933

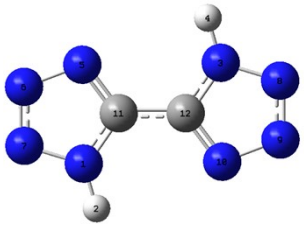
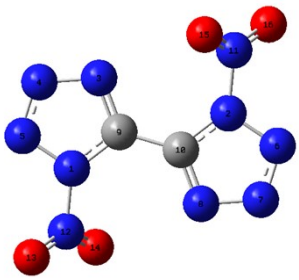
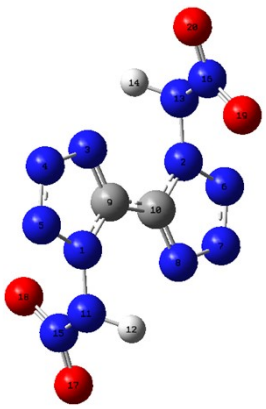
58	2.864	0.316733	-1.888700
59	2.915	0.311667	-1.821267
60	2.965	0.306500	-1.757367
61	3.015	0.301300	-1.696833
62	3.065	0.296067	-1.639400
63	3.116	0.290833	-1.584900
64	3.166	0.285600	-1.533167
65	3.216	0.280400	-1.484033
66	3.266	0.275200	-1.437300
67	3.317	0.270100	-1.392867
68	3.367	0.265033	-1.350567
69	3.417	0.260067	-1.310267
70	3.467	0.255167	-1.271867
71	3.518	0.250333	-1.235233
72	3.568	0.245633	-1.200267
73	3.618	0.240967	-1.166867
74	3.668	0.236400	-1.134933
75	3.719	0.231933	-1.104400
76	3.769	0.227567	-1.075200
77	3.819	0.223300	-1.047200
78	3.869	0.219100	-1.020400
79	3.920	0.215033	-0.994667
80	3.970	0.211033	-0.970000
81	4.020	0.207100	-0.946300
82	4.070	0.203300	-0.923533
83	4.121	0.199533	-0.901667
84	4.171	0.195900	-0.880600
85	4.221	0.192333	-0.860333
86	4.271	0.188867	-0.840800
87	4.322	0.185467	-0.822000
88	4.372	0.182100	-0.803867
89	4.422	0.178867	-0.786333
90	4.472	0.175700	-0.769467
91	4.523	0.172600	-0.753133
92	4.573	0.169567	-0.737367
93	4.623	0.166600	-0.722133
94	4.673	0.163700	-0.707367
95	4.724	0.160900	-0.693100
96	4.774	0.158133	-0.679300
97	4.824	0.155433	-0.665900
98	4.874	0.152733	-0.652933
99	4.925	0.150167	-0.640333
100	4.975	0.147633	-0.628133
101	5.025	0.145167	-0.616300
102	5.075	0.142767	-0.604800
103	5.126	0.140400	-0.593633
104	5.176	0.138067	-0.582800
105	5.226	0.135833	-0.572267
106	5.276	0.133600	-0.562000
107	5.327	0.131433	-0.552033
108	5.377	0.129333	-0.542333
109	5.427	0.127233	-0.532900
110	5.477	0.125200	-0.523700
111	5.528	0.123200	-0.514733
112	5.578	0.121300	-0.506000
113	5.628	0.119400	-0.497500
114	5.678	0.117500	-0.489200
115	5.729	0.115700	-0.481133
116	5.779	0.113900	-0.473233
117	5.829	0.112167	-0.465533
118	5.879	0.110433	-0.458033
119	5.930	0.108767	-0.450700
120	5.980	0.107100	-0.443533
121	6.030	0.105500	-0.436533
122	6.080	0.103933	-0.429700
123	6.131	0.102367	-0.423000
124	6.181	0.100833	-0.416467

125	6.231	0.099367	-0.410067
126	6.281	0.097900	-0.403833
127	6.332	0.096467	-0.397733
128	6.382	0.095067	-0.391733
129	6.432	0.093700	-0.385900
130	6.482	0.092367	-0.380167
131	6.533	0.091033	-0.374533
132	6.583	0.089733	-0.369067
133	6.633	0.088433	-0.363667
134	6.683	0.087200	-0.358400
135	6.734	0.085967	-0.353233
136	6.784	0.084767	-0.348200
137	6.834	0.083600	-0.343233
138	6.884	0.082433	-0.338367
139	6.935	0.081300	-0.333600
140	6.985	0.080200	-0.328933
141	7.035	0.079100	-0.324333
142	7.085	0.078033	-0.319833
143	7.136	0.076967	-0.315433
144	7.186	0.075933	-0.311100
145	7.236	0.074900	-0.306867
146	7.286	0.073900	-0.302700
147	7.337	0.072900	-0.298600
148	7.387	0.071967	-0.294600
149	7.437	0.070967	-0.290633
150	7.487	0.070067	-0.286767
151	7.538	0.069133	-0.282967
152	7.588	0.068233	-0.279233
153	7.638	0.067333	-0.275567
154	7.688	0.066467	-0.271967
155	7.739	0.065633	-0.268433
156	7.789	0.064767	-0.264933
157	7.839	0.063967	-0.261533
158	7.889	0.063133	-0.258167
159	7.940	0.062333	-0.254867
160	7.990	0.061533	-0.251600
161	8.040	0.060767	-0.248400
162	8.090	0.060000	-0.245267
163	8.141	0.059233	-0.242200
164	8.191	0.058500	-0.239133
165	8.241	0.057800	-0.236167
166	8.291	0.057067	-0.233233
167	8.342	0.056367	-0.230333
168	8.392	0.055667	-0.227500
169	8.442	0.054967	-0.224700
170	8.492	0.054333	-0.221933
171	8.543	0.053667	-0.219233
172	8.593	0.053000	-0.216567
173	8.643	0.052367	-0.213933
174	8.693	0.051733	-0.211367
175	8.744	0.051133	-0.208833
176	8.794	0.050500	-0.206333
177	8.844	0.049900	-0.203867
178	8.894	0.049333	-0.201433
179	8.945	0.048733	-0.199067
180	8.995	0.048133	-0.196700
181	9.045	0.047600	-0.194400
182	9.095	0.047033	-0.192100
183	9.146	0.046467	-0.189867
184	9.196	0.045967	-0.187667
185	9.246	0.045433	-0.185467
186	9.296	0.044867	-0.183333
187	9.347	0.044367	-0.181233
188	9.397	0.043833	-0.179133
189	9.447	0.043367	-0.177100
190	9.497	0.042867	-0.175067
191	9.548	0.042400	-0.173067

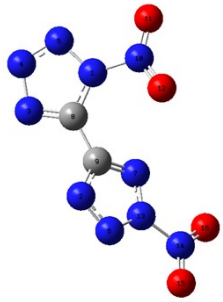
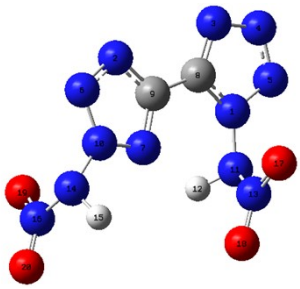
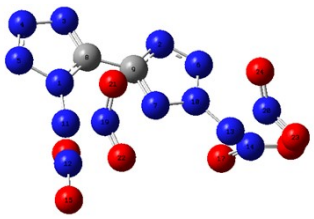
192	9.598	0.041900	-0.171100
193	9.648	0.041433	-0.169167
194	9.698	0.040967	-0.167267
195	9.749	0.040500	-0.165400
196	9.799	0.040033	-0.163533
197	9.849	0.039600	-0.161733
198	9.899	0.039167	-0.159933
199	9.950	0.038733	-0.158167
200	10.000	0.038300	-0.156400

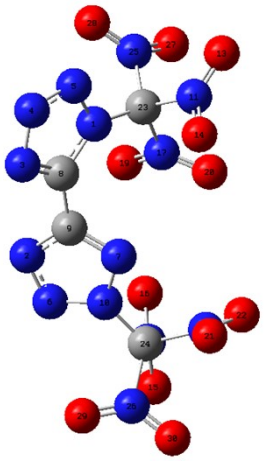
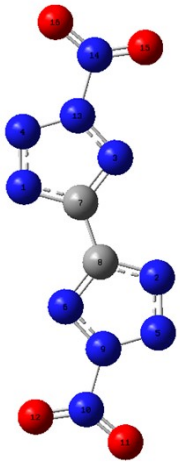
[a] *Inorg. Chem.* **2014**, *53(7)*, 3579-3585. [b] Column 1: Point index; Column 2: Scanning distance in Angstrom; Column 3: In-plane component of NICS; Column 4: Out-of-plane component of NICS.

Table **S6** Geometric optimization structure (at M06-2X/6-311g+(2d,p) level)

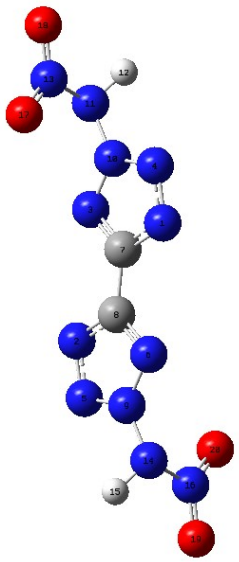
No.	geometric optimization structure			
I		N	-1.32554100	-0.90719500	0.91582500
		H	-1.25409400	-0.74692100	1.91098600
		N	1.32554100	0.90719500	-0.91582500
		H	1.25409400	0.74692100	-1.91098600
		N	-1.02877900	-0.91145200	-1.21239800
		N	-2.08811800	-1.68052600	-0.87967500
		N	-2.27413400	-1.68523900	0.38748900
		N	2.27413400	1.68523900	-0.38748900
		N	2.08811800	1.68052600	0.87967500
		N	1.02877900	0.91145200	1.21239800
		C	-0.56747900	-0.43942600	-0.08179300
		C	0.56747900	0.43942600	0.08179300
I-01		N	-1.56253900	-0.78116900	0.68795900
		N	1.56253900	0.78116900	-0.68795900
		N	-0.64699500	-1.23105800	-1.19191000
		N	-1.76502600	-1.97331000	-1.01412900
		N	-2.32130000	-1.71114200	0.10336600
		N	2.32130000	1.71114200	-0.10336600
		N	1.76502600	1.97331000	1.01412900
		N	0.64699500	1.23105800	1.19191000
		C	-0.51392100	-0.49728400	-0.12065200
		C	0.51392100	0.49728400	0.12065200
		N	1.84241900	0.44308100	-2.08708300
		N	-1.84241900	-0.44308100	2.08708300
		O	-2.97797300	-0.16763300	2.29896500
		O	-0.89888000	-0.52072000	2.80593600
		O	0.89888000	0.52072000	-2.80593600
		O	2.97797300	0.16763300	-2.29896500
I-02		N	-1.81730400	0.34269500	0.15811600
		N	1.81730400	-0.34269500	-0.15811600
		N	-0.74536700	-0.04298600	-1.66865300
		N	-2.07216100	0.14959900	-1.91623400
		N	-2.71526600	0.36813900	-0.84225900
		N	2.71526600	-0.36813900	0.84225900
		N	2.07216100	-0.14959900	1.91623400
		N	0.74536700	0.04298600	1.66865300
		C	-0.60938100	0.06810400	-0.37875100
		C	0.60938100	-0.06810400	0.37875100
		N	-2.21191400	0.44496400	1.45818100
		H	-1.63560400	1.09390000	1.99395200
		N	2.21191400	-0.44496400	-1.45818100
		H	1.63560400	-1.09390000	-1.99395200
		N	-2.13186900	-0.82557200	2.15580200
		N	2.13186900	0.82557200	-2.15580200

	O	-2.18216300	-0.71287600	3.34363300
	O	-2.06836800	-1.80991900	1.47775200
	O	2.06836800	1.80991900	-1.47775200
	O	2.18216300	0.71287600	-3.34363300
I-03	N	-1.84107300	0.22613500	0.21530400
	N	1.84107300	-0.22613500	-0.21530400
	N	-0.74557300	0.31728400	-1.63242000
	N	-2.07657000	0.53026000	-1.84860200
	N	-2.73314500	0.48133100	-0.76624500
	N	2.73314500	-0.48133100	0.76624500
	N	2.07657000	-0.53026000	1.84860200
	N	0.74557300	-0.31728400	1.63242000
	C	-0.61511000	0.12904100	-0.35452800
	C	0.61511000	-0.12904100	0.35452800
	N	-2.26207100	0.09506900	1.49197600
	N	2.26207100	-0.09506900	-1.49197600
	N	-2.11279200	-1.32602000	1.98540800
	N	2.11279200	1.32602000	-1.98540800
	O	-1.68866700	-2.08831600	1.17253200
	O	-2.51153700	-1.50304900	3.08428000
	O	2.51153700	1.50304900	-3.08428000
	O	1.68866700	2.08831600	-1.17253200
	N	-1.60835500	1.12967500	2.39371200
	N	1.60835500	-1.12967500	-2.39371200
	O	-1.64641200	0.90016800	3.54983700
	O	-1.20098900	2.07089800	1.78907900
	O	1.20098900	-2.07089800	-1.78907900
	O	1.64641200	-0.90016800	-3.54983700
I-04	N	-1.65142400	-0.66052700	0.58540800
	N	1.65142400	0.66052700	-0.58540800
	N	-0.49994100	-1.37148200	-1.08812600
	N	-1.63742900	-2.09673400	-0.95786900
	N	-2.32850000	-1.69524100	0.02412600
	N	2.32850000	1.69524100	-0.02412600
	N	1.63742900	2.09673400	0.95786900
	N	0.49994100	1.37148200	1.08812600
	C	-0.51480900	-0.49169200	-0.13023000
	C	0.51480900	0.49169200	0.13023000
	N	-3.46448900	-0.64722800	2.14849100
	N	3.46448900	0.64722800	-2.14849100
	O	-3.35609000	-1.47905200	3.00192000
	O	-4.43472100	-0.27489800	1.55612900
	O	4.43472100	0.27489800	-1.55612900
	O	3.35609000	1.47905200	-3.00192000
	N	-1.16733200	-0.09295700	2.91079100
	N	1.16733200	0.09295700	-2.91079100
	O	-0.32758900	-0.94044700	2.78430900
	O	-1.38110600	0.63065300	3.83361000
	O	1.38110600	-0.63065300	-3.83361000
	O	0.32758900	0.94044700	-2.78430900
	C	-2.14659500	0.02206700	1.71056600
	C	2.14659500	-0.02206700	-1.71056600
	N	-2.49580500	1.49248200	1.38707400
	N	2.49580500	-1.49248200	-1.38707400
	O	-2.25118900	1.84545000	0.26612300
	O	-3.00849500	2.10098600	2.27762300
	O	3.00849500	-2.10098600	-2.27762300

		O	2.25118900	-1.84545000	-0.26612300
I-05		N	-2.16758000	0.14629000	-0.07073000
		N	0.87675600	-1.59993900	0.94097600
		N	-1.88261400	-1.94214300	-0.43290300
		N	-3.19088300	-1.59329700	-0.58856400
		N	-3.37161200	-0.35329200	-0.37665700
		N	2.11418200	-1.24796300	0.85959600
		N	0.96689400	0.11792400	-0.47632900
		C	-1.24973600	-0.85629200	-0.09862200
		C	0.18927100	-0.75596700	0.12427000
		N	-2.03741800	1.51839100	0.35773400
		O	-2.94889000	2.22347400	0.07481800
		O	-1.02235300	1.75105700	0.94711800
		N	2.12846200	-0.23320900	0.01457000
		N	3.37181400	0.45909800	-0.34841300
		O	4.33633800	0.03635800	0.19949700
		O	3.22325200	1.33542900	-1.13503800
I-06		N	2.20879200	-0.17028800	-0.59574400
		N	-0.32717000	2.28321700	0.62776700
		N	2.59226100	1.87849000	-0.05776000
		N	3.73150200	1.26259300	-0.48367100
		N	3.52031700	0.04898500	-0.79469100
		N	-1.55661400	2.00225000	0.87162600
		N	-0.58552000	0.10955300	0.22867800
		C	1.65801400	0.97763000	-0.12248500
		C	0.25918700	1.11808300	0.23773000
		N	-1.69279000	0.70441600	0.64143500
		N	1.67887700	-1.40624900	-0.79964500
		H	0.86472900	-1.40996100	-1.41029900
		N	1.28684400	-2.06479900	0.41612700
		N	-2.89756600	0.08727200	0.74866200
		H	-2.84460000	-0.78999200	1.26381400
		N	-3.47712500	-0.20926000	-0.54414900
		O	1.78656400	-1.67663600	1.43101700
		O	0.51171200	-2.96401900	0.24206200
		O	-3.10922900	0.46095800	-1.46209400
		O	-4.30104500	-1.07750000	-0.50541500
I-07		N	-2.72975800	0.30339200	0.10154700
		N	0.40651400	2.34624500	-0.09347800
		N	-2.58027400	2.44939800	0.17572700
		N	-3.88477900	2.04567300	0.25217800
		N	-3.98887800	0.78561300	0.21282100
		N	1.59277700	1.87280800	-0.14115500
		N	0.21516700	0.12729500	-0.01783100
		C	-1.87538300	1.36570200	0.08098200
		C	-0.43062300	1.26965800	-0.00980200
		N	1.46449400	0.54593000	-0.10289600
		N	-2.54129500	-1.02941600	0.02555800
		N	-2.06136900	-1.46934100	-1.33075900
		N	2.50887000	-0.31558900	-0.08759700
		N	3.46208400	0.04070800	-1.20892600
		O	-2.01194300	-2.64394800	-1.47155100
		O	-1.86834200	-0.58147600	-2.10456600
		O	2.89617400	0.18025300	-2.24312500
		O	4.61024800	0.09672500	-0.92479600
		N	-1.69794900	-1.54354200	1.16270300
		N	3.20105100	-0.32368000	1.26017600

	O	-1.73719300	-0.83618400	2.11984200
	O	-1.15750300	-2.58085000	0.98595400
	O	4.03841200	-1.15736600	1.34194900
	O	2.76382900	0.44027000	2.06085100
I-08 	N	-2.48714200	-0.95132500	0.10802700
	N	0.66808500	-2.17861600	-1.23845000
	N	-1.91628600	-3.01879000	0.33933000
	N	-3.23218400	-2.85136000	0.63784300
	N	-3.58397000	-1.64415300	0.52469700
	N	1.84275000	-1.67700100	-1.18914700
	N	0.65169200	-0.68876400	0.41587800
	C	-1.45491000	-1.84600500	0.03318400
	C	-0.05165600	-1.56402500	-0.25690000
	N	1.83027900	-0.79949200	-0.18007800
	N	-3.01639800	1.03966000	1.35193300
	N	3.23341200	0.85679700	-1.24109600
	O	-3.91472100	1.82853500	1.36688800
	O	-2.34901800	0.62016800	2.25525000
	O	4.39025600	1.05405400	-1.47470400
	O	2.25903800	1.18975500	-1.85152700
	N	-1.34616900	1.12020700	-0.50076700
	N	2.56023200	1.07336800	1.15819000
	O	-0.97603000	0.72156900	-1.57532600
	O	-0.86629100	1.95571200	0.20354300
	O	2.42672100	0.56873800	2.23607600
	O	2.46724700	2.21944500	0.82891600
	C	-2.62733000	0.44209400	-0.01860900
	C	2.91793100	0.07298700	0.05329600
	N	-3.68213200	0.87029700	-1.07190500
	N	4.19709300	-0.64254900	0.51285200
	O	-3.59661400	2.02609200	-1.38350600
	O	-4.43895900	0.03184000	-1.45754000
	O	4.27813100	-1.80471200	0.23676100
	O	4.97786000	0.06527000	1.08304800
I-09 	N	1.11330700	1.50106200	0.00005100
	N	-1.11328400	-1.50101800	-0.00039500
	N	1.70278600	-0.64925400	-0.00009000
	N	2.40004900	1.47086500	0.00006600
	N	-2.39999900	-1.47086600	-0.00030700
	N	-1.70281300	0.64928700	0.00017000
	C	0.69894800	0.20152200	-0.00003900
	C	-0.69896000	-0.20144400	-0.00008300
	N	-2.71318900	-0.18613400	0.00006000
	N	-4.10290200	0.27139000	0.00008200
	O	-4.90259700	-0.60814700	0.00047300
	O	-4.22516600	1.45275600	-0.00025900
	N	2.71317600	0.18614500	-0.00005500
	N	4.10290000	-0.27142800	0.00005600
	O	4.22512600	-1.45279600	0.00032200
	O	4.90261800	0.60808500	-0.00012700

I-10



N	-1.82555900	-0.38232600	0.08684600
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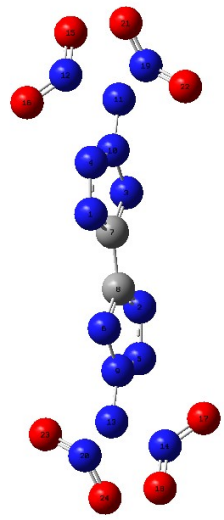
N	-0.71236300	0.63624000	-1.55196300
N	-2.68341900	-0.10161000	-0.82670100
N	2.68341900	0.10161000	0.82670100
N	0.71236300	-0.63624000	1.55196300
C	-0.62290800	0.06660300	-0.37023100
C	0.62290800	-0.06660300	0.37023100
N	2.00341000	-0.51667900	1.78591600
N	-2.00341000	0.51667900	-1.78591600
N	-2.57095100	0.92064700	-2.95429100
H	-3.46879300	1.37676400	-2.80550000
N	-2.80365600	-0.18385500	-3.85915100
N	2.57095100	-0.92064700	2.95429100
H	3.46879300	-1.37676400	2.80550000
N	2.80365600	0.18385500	3.85915100
O	-2.12087700	-1.15204000	-3.71150900
O	-3.63789000	0.05049100	-4.68828700
O	3.63789000	-0.05049100	4.68828700
O	2.12087700	1.15204000	3.71150900

I-11



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N	-0.61697600	0.57795600	-1.61053100
N	-2.64612400	-0.07832700	-0.94323400
N	2.64612400	0.07832700	0.94323400
N	0.61697600	-0.57795600	1.61053100
C	-0.60114400	0.06396100	-0.40428600
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N	1.90167000	-0.47162100	1.90333800
N	-1.90167000	0.47162100	-1.90333800
N	-2.39135400	0.85269400	-3.10640200
N	-2.67888100	-0.33606500	-3.99520900
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N	2.67888100	0.33606500	3.99520900
O	-2.97210000	-0.02434800	-5.10075600
O	-2.50057800	-1.40274800	-3.49785700
O	2.50057800	1.40274800	3.49785700
O	2.97210000	0.02434800	5.10075600
N	-3.62436700	1.69716500	-2.89635300
N	3.62436700	-1.69716500	2.89635300
O	-4.57355200	1.41817700	-3.54925200
O	-3.44111900	2.56449000	-2.10584100
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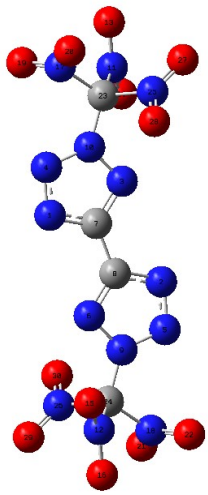
O	4.57355200	-1.41817700	3.54925200

I-12



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N	-0.67957500	0.35467800	-1.64832100
N	-2.65511100	0.65660300	-0.64761800
N	2.65511100	-0.65660300	0.64761800
N	0.67957500	-0.35467800	1.64832100
C	-0.61144900	0.17516100	-0.35235800
C	0.61144900	-0.17516100	0.35235800
N	1.96673900	-0.62679800	1.79961300
N	-1.96673900	0.62679800	-1.79961300
N	-2.45697100	-0.03397400	-4.12865900
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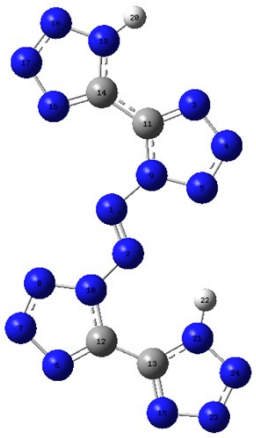
O	-3.22168700	0.15310100	-5.03244500
O	-1.66953500	-0.92087800	-3.96576700
O	1.66953500	0.92087800	3.96576700
O	3.22168700	-0.15310100	5.03244500
N	-3.97018800	1.43299500	-2.86985000
N	3.97018800	-1.43299500	2.86985000
O	-4.68517400	0.50447600	-2.62458100
O	-4.23703400	2.59073200	-3.01340000
O	4.23703400	-2.59073200	3.01340000
O	4.68517400	-0.50447600	2.62458100
C	-2.49607800	1.04714000	-3.03587200
C	2.49607800	-1.04714000	3.03587200
N	-1.71052400	2.27791600	-3.54137100
N	1.71052400	-2.27791600	3.54137100
O	-1.49797900	2.32960000	-4.71787000
O	-1.41401900	3.05090000	-2.67571100
O	1.49797900	-2.32960000	4.71787000
O	1.41401900	-3.05090000	2.67571100

II



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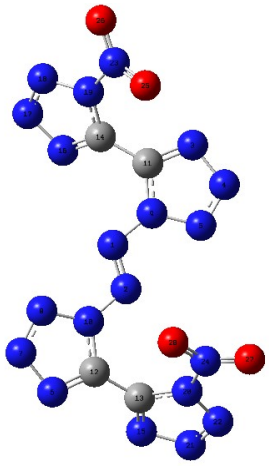
N	-1.66287600	2.93247600	0.00002100
N	-0.69227000	2.11061400	-0.00011300
N	3.21341300	-2.39018800	0.00006600
N	2.09304900	-3.17188400	0.00005200
N	1.02524200	-2.48520100	-0.00002100
N	-1.24334600	0.87706100	-0.00014100
N	1.43005300	-1.19427100	-0.00005800
C	-2.58741800	1.01323800	-0.00006200
C	2.79100900	-1.16056500	0.00005100
C	3.59510000	0.04932100	0.00003900
C	-3.59454200	-0.02603300	-0.00001600
N	4.90545700	0.07897300	0.00019200
N	-3.44830900	-1.32671400	-0.00025900
N	-4.70053200	-1.82896400	-0.00012700
N	-5.57657900	-0.89075600	0.00023100
N	-4.90577300	0.25762600	0.00029500
H	-5.37321200	1.15440800	0.00059300
N	3.14411400	1.31759700	-0.00009200
H	2.19932400	1.68219200	-0.00023600
N	5.24125700	1.38142500	0.00010500
N	4.19831200	2.13017200	-0.00003500

II-01



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N	0.93387800	-0.32604900	-0.18387100
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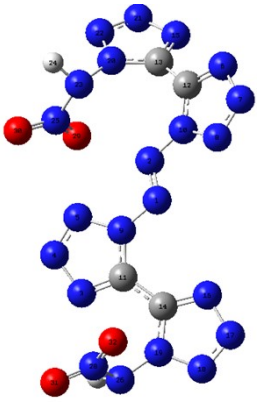
N	-1.33416700	2.70744700	-0.87268500
N	-0.37273500	1.91506100	-0.60889500
N	3.29340200	-2.68250900	0.69656800
N	2.11532400	-3.29785400	1.01373700
N	1.10964100	-2.56843300	0.74369300
N	-0.92721300	0.69795500	-0.45634700
N	1.61168100	-1.43104200	0.22614500
C	-2.26284800	0.81462300	-0.63136900
C	2.96305900	-1.52279500	0.21704100
C	3.86118100	-0.50409200	-0.31434100
C	-3.18814400	-0.30758000	-0.63036800
N	4.74143500	-0.69930900	-1.25074100
N	-3.01205100	-1.42392200	-1.27730500
N	-4.14420100	-2.15550200	-1.09067800
N	-4.99052200	-1.52780600	-0.37679400
N	-4.42389300	-0.35573800	-0.07548200
N	3.91708100	0.81437500	0.01810100
N	5.34188000	0.50496300	-1.46926400
N	4.85879400	1.41088200	-0.71969000
N	-5.06431900	0.55207600	0.85833100
N	3.22176800	1.53902100	1.05094600
O	-4.30803200	1.31038600	1.38672400
O	-6.23563000	0.40805000	0.97003900
O	3.38236200	2.71182000	1.04824700
O	2.57479400	0.83802900	1.77932400

II-02



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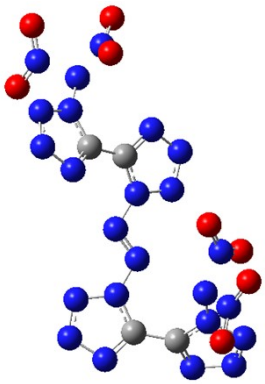
N	2.51919700	1.63403700	0.55113000
N	1.42201900	2.37878200	0.25759200
N	0.41753000	1.64260300	0.00394500
N	-3.59582800	-2.79618900	-0.80611200
N	-2.45527600	-3.44379600	-1.17540000
N	-1.42202800	-2.73041300	-0.98486800
N	0.83970600	0.36799600	0.12522500
N	-1.86768500	-1.56312700	-0.47663300
C	2.14855200	0.38482200	0.45268100
C	-3.22169500	-1.62610600	-0.37873300
C	-4.12625200	-0.61425500	0.15219700
C	3.00874700	-0.75246600	0.69384500
N	-5.13606900	-0.86835100	0.93582500
N	2.68477400	-1.99023100	0.92463500
N	3.86389400	-2.65063600	1.09600500
N	4.85895500	-1.86573100	0.98222500
N	4.35908600	-0.64391900	0.74770600
N	-4.15287100	0.70503200	-0.14741500
N	-5.77515300	0.31566300	1.11977900
N	-5.20031000	1.25732300	0.48677300
N	-3.27645200	1.43502500	-0.89217300
H	-3.75686700	2.02122600	-1.57392700
N	-2.49487100	2.34804000	-0.06422400
N	5.18574600	0.41004500	0.49513200
H	4.92981800	1.24227400	1.02658900
N	5.15962300	0.80772600	-0.89683300
O	-2.34858300	2.04084500	1.07894200

	O	-2.06269000	3.28007100	-0.67691800
	O	5.63399200	1.88874200	-1.08630900
	O	4.71206100	0.01911400	-1.67921400
II-03 	N	0.20797000	-1.00493200	-0.31701600
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	N	-2.17712000	1.40024500	-1.06425200
	N	-1.11276100	1.76355300	-1.82892700
	N	-0.12180700	0.98635800	-1.65346700
	N	3.87235200	-3.17590600	0.13765200
	N	2.72190700	-3.84366600	0.43725100
	N	1.69121700	-3.12117900	0.25836300
	N	-0.52014500	0.06837900	-0.75078700
	N	2.14833900	-1.92958700	-0.17340200
	C	-1.79977400	0.33932300	-0.40807400
	C	3.50296800	-1.99133000	-0.24801100
	C	4.37606700	-0.90921700	-0.67729500
	C	-2.58646600	-0.37781200	0.57442800
	N	5.39922000	-1.00269100	-1.46896000
	N	-2.16858900	-0.99573700	1.63937700
	N	-3.29019300	-1.42714700	2.28481300
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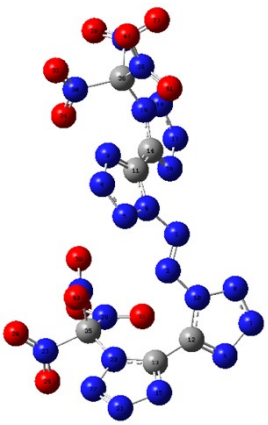
II-04 	N	0.36970500	-1.60545100	-0.53951800
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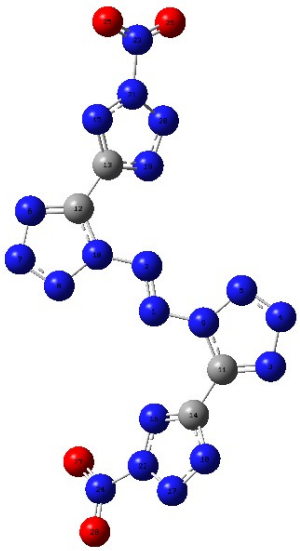
II-05



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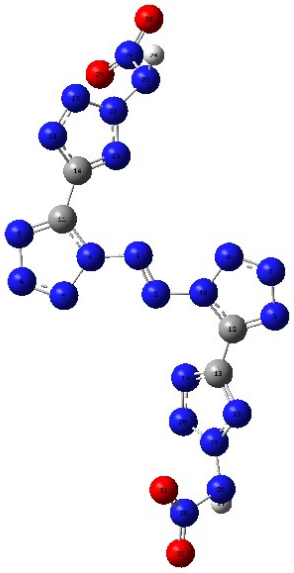

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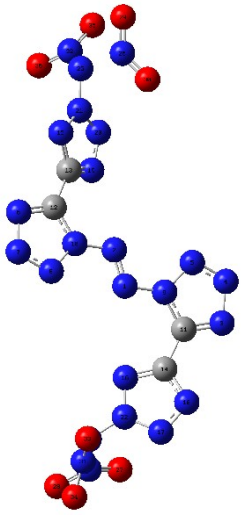
II-07



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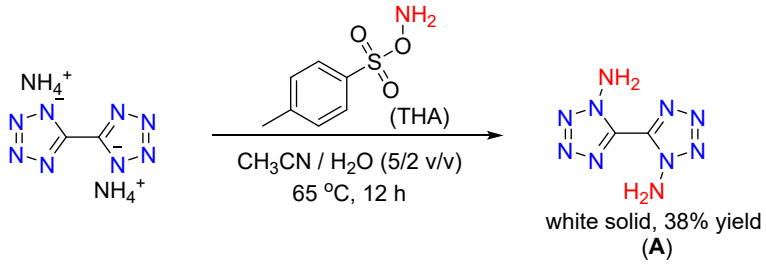
Part II Experimental study details



A magnetic stir bar was placed in a dried 50 mL round-bottom flask, followed by the addition of 120 mg (0.7 mmol) of 5,5'-diazomethane disodium salt. Then, 25 mL of acetonitrile, 10 mL of water and a pre-prepared dichloromethane solution of THA were introduced successively. The reaction mixture was stirred at room temperature for 12 h and the progress was monitored by TLC using EA as the eluent. After completion, acetonitrile was removed under reduced pressure. The aqueous phase was extracted repeatedly with ethyl acetate (monitored by TLC until complete extraction). The combined organic extracts were dried over anhydrous Na_2SO_4, filtered and concentrated to afford a pale-yellow crude solid. The product was further purified by silica gel column chromatography with a mixture of PE and EA (4/3 v/v) as the eluent. Finally, 44.9 mg of the derivative **A** was obtained, yielding 38%.

1,1'-Diamino-5,5'-biquinolizole (**A**):

^{1}H NMR (500 MHz, DMSO-d_6) δ 7.44 (s, 4H) ppm.

^{13}C NMR (126 MHz, DMSO-d_6) δ 141.2 ppm.

IR (KBr): 3342.22, 3233.35, 3163.38, 2920.31, 2849.72, 1615.35, 1587.11, 1388.24, 1266.70, 1129.21, 1031.00, 993.55, 921.13, 895.35, 713.04, 705.49, 689.72, 666.39, 463.22 cm^{-1}.

Elemental analysis $C_2H_4N_{10}$ (168.06) Calculated values: C 14.29, H 2.40, N 83.31%, Measured values: C 13.89, H 4.56, N 81.55%.

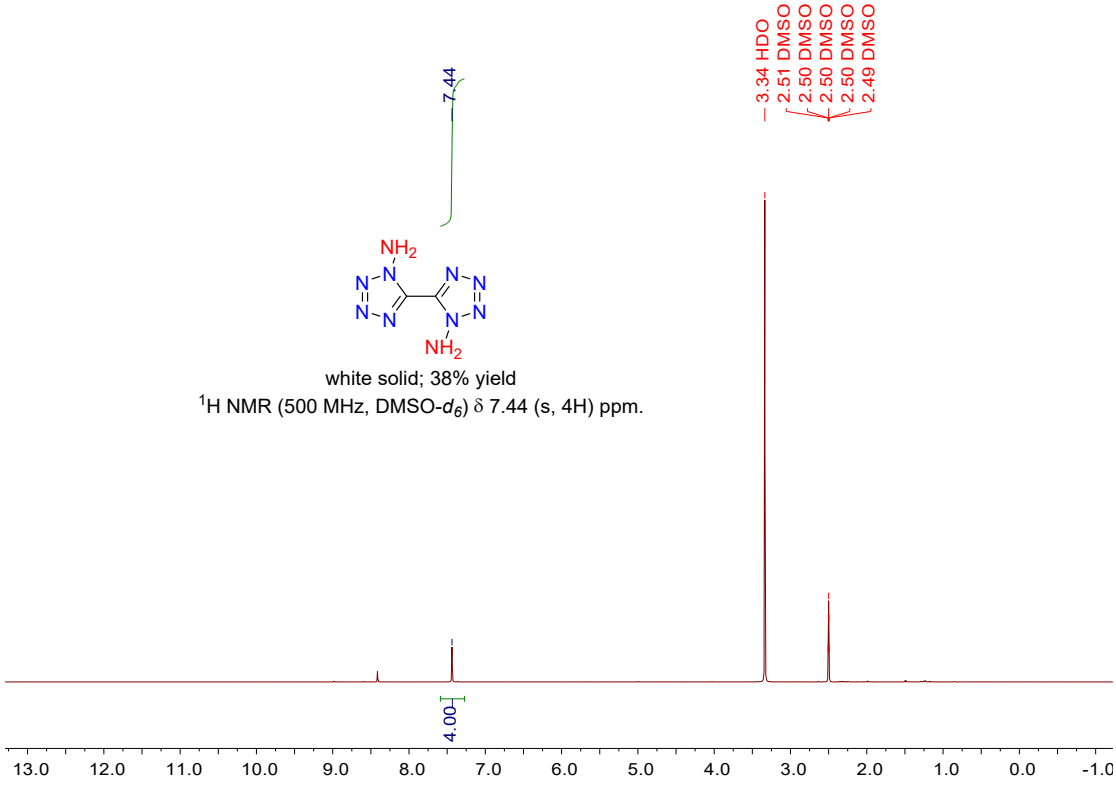


Fig. **S8** ^{1}H NMR (DMSO-d_6, 500 MHz) map of derivative **A**

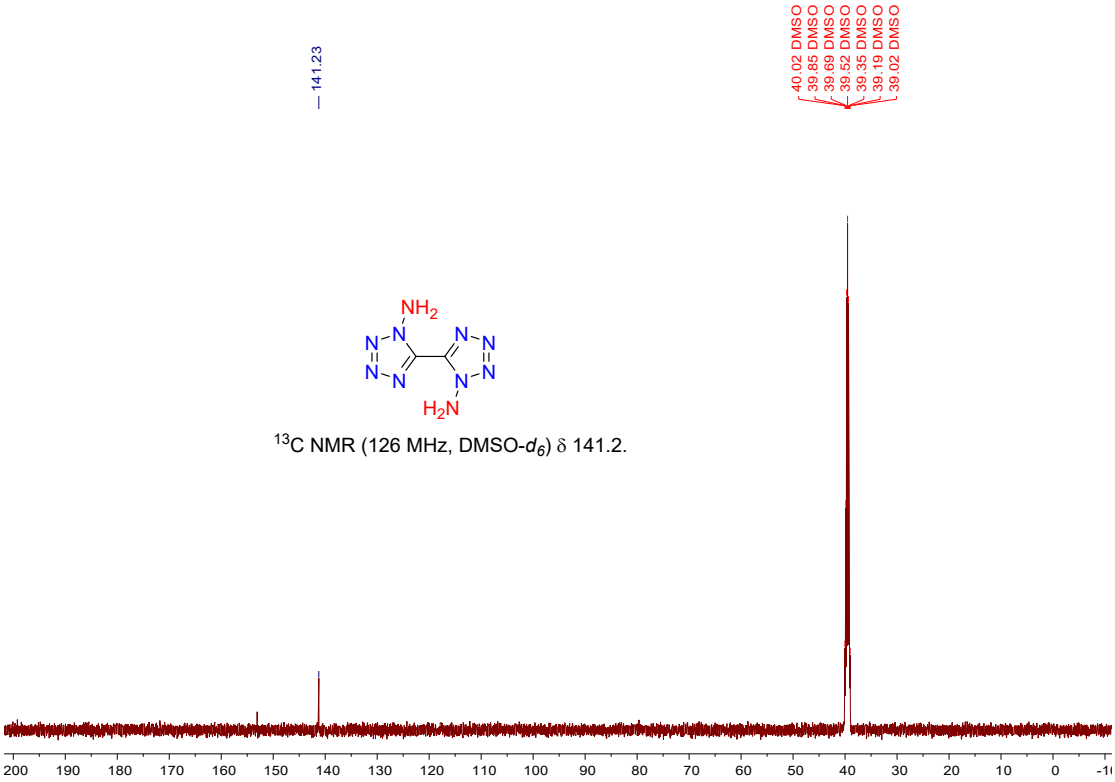


Fig. **S9** ^{13}C NMR (DMSO-d_6, 126 MHz) map of derivative **A**

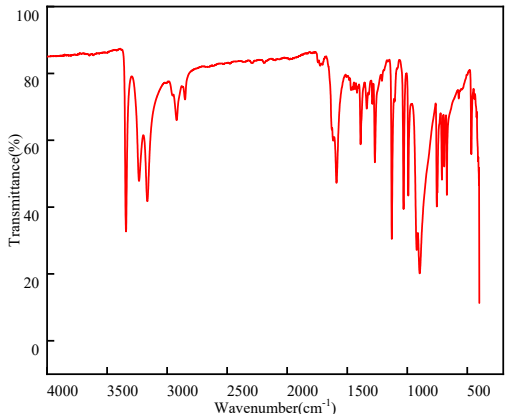


Fig. **S10** IR map of derivative **A**

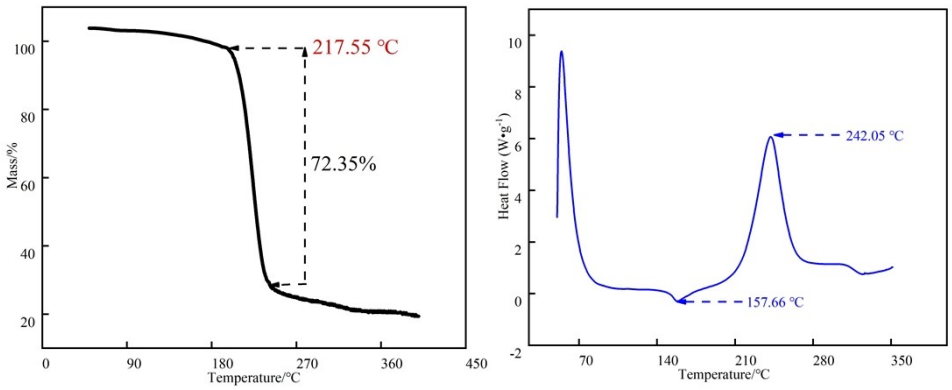
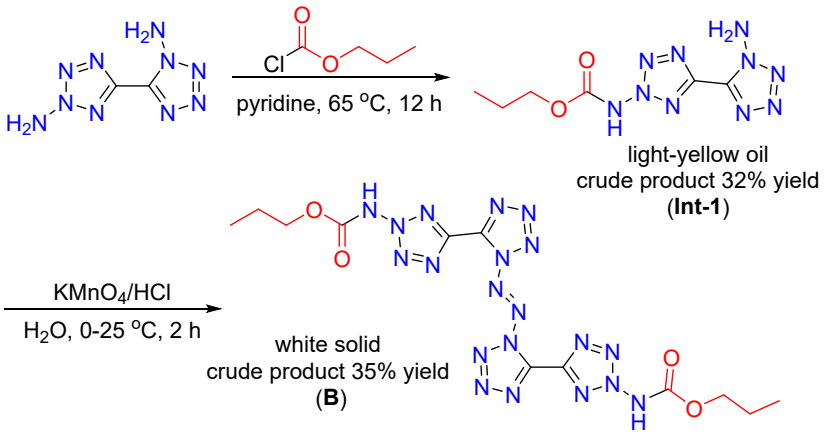


Fig. **S11** TG map (left) and DSC map (right) of derivative **A**



Under a N_2 atmosphere at 65 °C, 0.60 g (3.5 mmol) of 1,2-diamino-5,5'-bistetrazole was dissolved in 5 mL of pyridine. Then 0.96 g (7.9 mmol) of propyl chloroformate was added. The reaction was maintained under the same conditions for 12 h. After completion, the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using a mixture of PE and EA (3/2 v/v) as the eluent, affording a light-yellow oil intermediate (**Int-1**, crude product 32% yield). At 0 °C, this light-yellow oil intermediate (180 g, 0.7 mmol) was added to 5 mL of HCl, followed by the addition of $KMnO_4$ (0.33 g, 2.1 mmol). The reaction mixture was then warmed to 25 °C and stirred for 2 h. The reaction was quenched by adding an aqueous solution of H_2O_2, resulting in the precipitation of a white solid, which corresponded to the desire product (derivative **B**). The crude product (35% yield) was collected by filtration and further purified by recrystallization from methanol to yield the pure final product.

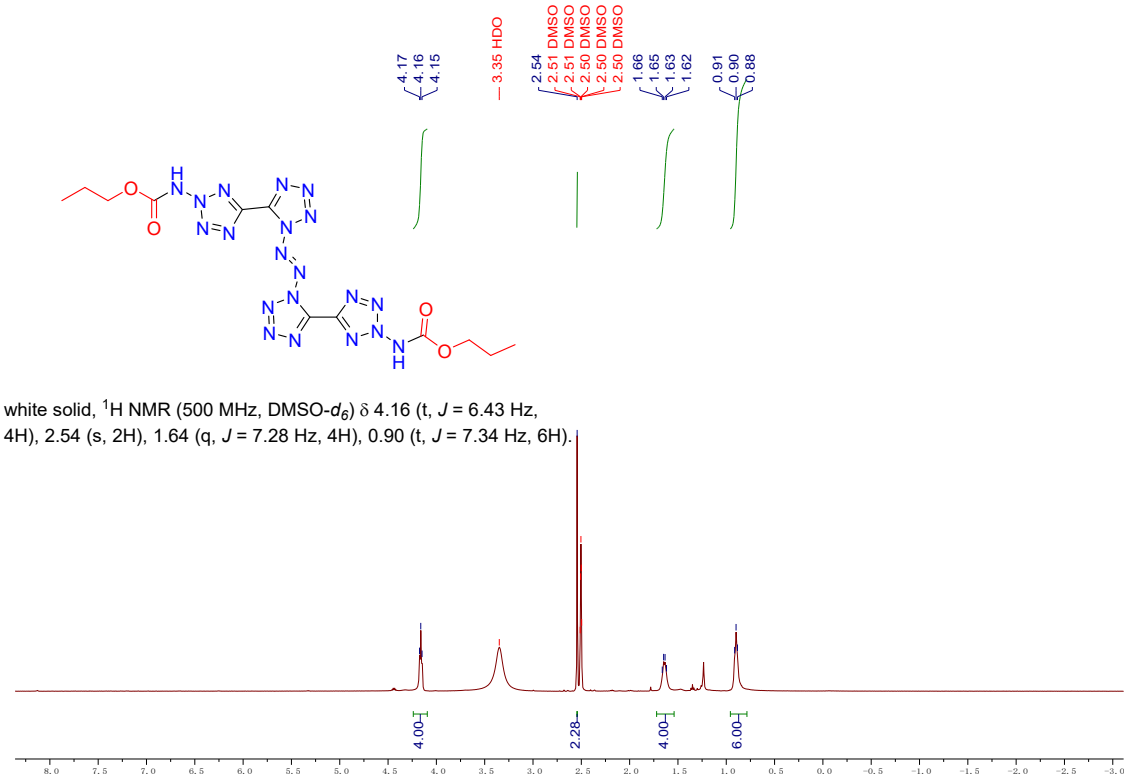
propyl (1-amino-1*H*,2'*H*-[5,5'-bitetrazol]-2'-yl)carbamate (**Int-1**)

^{13}C NMR (126 MHz, DMSO-d_6) δ 152.0, 143.3, 68.8, 22.0, 10.4 ppm.

dipropyl (diazene-1,2-diylbis((1H,2'H-[5,5'-bitetrazole]-1,2'-diyl)))(E)-dicarbamate (**B**)

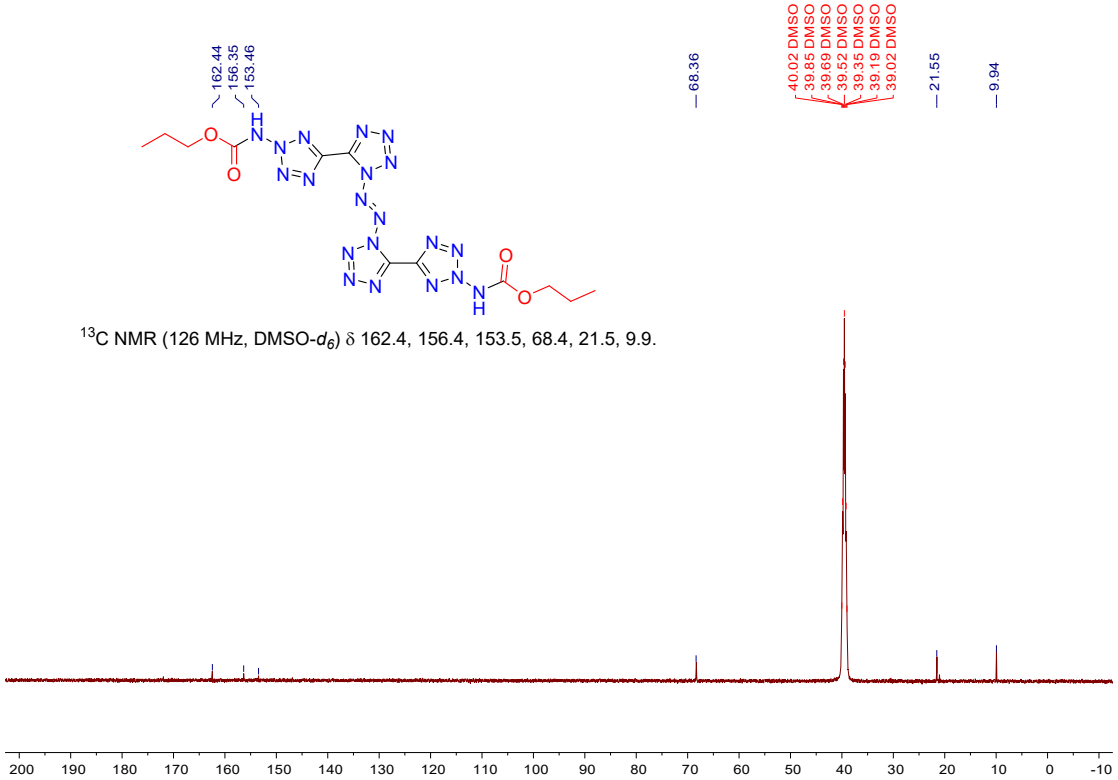
^{1}H NMR (500 MHz, DMSO-d_6) δ 4.16 (t, J = 6.43 Hz, 4H), 2.54 (s, 2H), 1.64 (q, J = 7.28 Hz, 4H), 0.90 (t, J = 7.34 Hz, 6H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 162.4, 156.4, 153.5, 68.4, 21.5, 9.9 ppm.



white solid, ^{1}H NMR (500 MHz, DMSO-d_6) δ 4.16 (t, J = 6.43 Hz, 4H), 2.54 (s, 2H), 1.64 (q, J = 7.28 Hz, 4H), 0.90 (t, J = 7.34 Hz, 6H).

Fig. **S12** ^{1}H NMR (DMSO-d_6, 500 MHz) map of derivative **B**



^{13}C NMR (126 MHz, DMSO-d_6) δ 162.4, 156.4, 153.5, 68.4, 21.5, 9.9.

Fig. **S13** ^{13}C NMR (DMSO-d_6, 126 MHz) map of derivative **B**

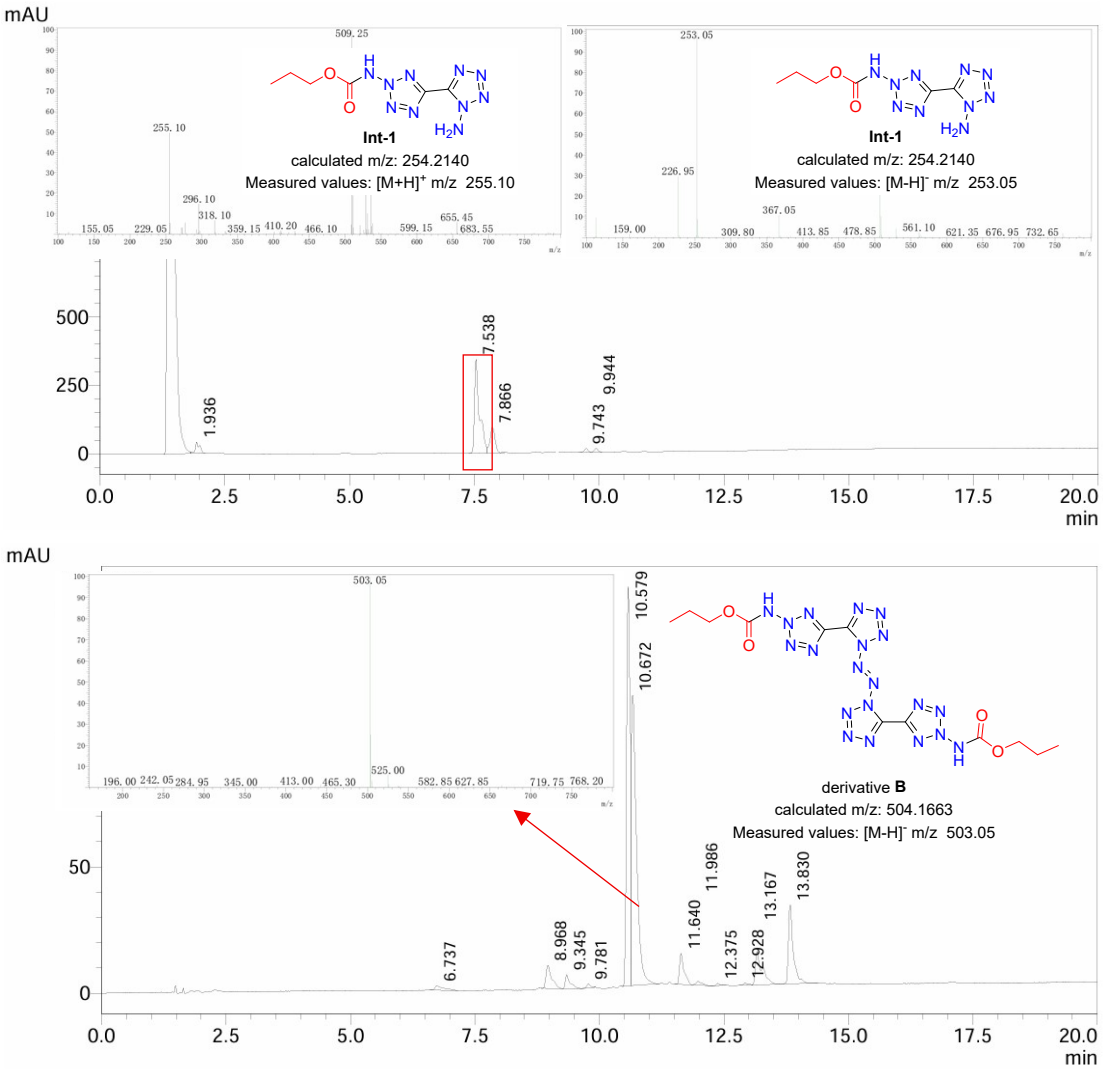
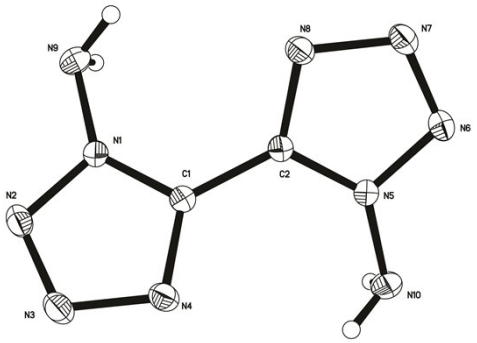


Fig. **S14** LC-MS analysis of **Int-1** and derivative **B**

Part III X-ray diffraction analysis details

Table **S7** Crystal data and structure refinement for derivative **A**



CCDC deposition number	2538870
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Formula weight	168.15
Temperature	296(2) K

Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 6.2039(4) Å	α= 90°.
	b = 10.1051(6) Å	β= 104.096(2)°.
	c = 10.3445(6) Å	γ = 90°.
Volume	628.98(7) $Å^3$	
Z	4	
Density (calculated)	1.776 Mg/m^3	
Absorption coefficient	0.141 mm^{-1}	
F(000)	344	
Crystal size	0.250 x 0.100 x 0.080 mm^3	
Theta range for data collection	2.861 to 27.500°.	
Index ranges	-8<=h<=7, -12<=k<=13, -11<=l<=13	
Reflections collected	6110	
Independent reflections	1425 [R(int) = 0.0249]	
Completeness to theta = 25.242°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6760	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1425 / 0 / 121	
Goodness-of-fit on F^2	1.072	
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0849	
R indices (all data)	R1 = 0.0377, wR2 = 0.0882	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.280 and -0.196 $e.Å^{-3}$	

Table **S8** Bond lengths [Å] and angles [°] for derivative **A**

Bond lengths [Å		Angles [°]	
C(1)-N(4)	1.3179(14)	N(4)-C(1)-N(1)	108.97(10)
C(1)-N(1)	1.3409(14)	N(4)-C(1)-C(2)	126.37(10)
C(1)-C(2)	1.4516(15)	N(1)-C(1)-C(2)	124.54(10)
C(2)-N(8)	1.3186(14)	N(8)-C(2)-N(5)	108.89(9)
C(2)-N(5)	1.3407(14)	N(8)-C(2)-C(1)	126.03(10)
N(1)-N(2)	1.3385(14)	N(5)-C(2)-C(1)	124.96(10)
N(1)-N(9)	1.3902(14)	N(2)-N(1)-C(1)	108.18(9)
N(2)-N(3)	1.2936(15)	N(2)-N(1)-N(9)	119.06(9)
N(3)-N(4)	1.3619(14)	C(1)-N(1)-N(9)	132.76(10)
N(5)-N(6)	1.3387(13)	N(3)-N(2)-N(1)	106.73(9)

N(5)-N(10)	1.3903(14)	N(2)-N(3)-N(4)	110.87(9)
N(6)-N(7)	1.2936(14)	C(1)-N(4)-N(3)	105.24(9)
N(7)-N(8)	1.3602(13)	N(6)-N(5)-C(2)	108.25(9)
N(9)-H(9A)	0.911(18)	N(6)-N(5)-N(10)	118.76(9)
N(9)-H(9B)	0.871(18)	C(2)-N(5)-N(10)	132.99(10)
N(10)-H(10A)	0.903(19)	N(7)-N(6)-N(5)	106.63(9)
N(10)-H(10B)	0.864(19)	N(6)-N(7)-N(8)	110.97(9)
		C(2)-N(8)-N(7)	105.26(9)
		N(1)-N(9)-H(9A)	106.5(11)
		N(1)-N(9)-H(9B)	107.9(11)
		H(9A)-N(9)-H(9B)	109.5(16)
		N(5)-N(10)-H(10A)	107.9(11)
		N(5)-N(10)-H(10B)	108.3(12)
		H(10A)-N(10)-H(10B)	110.7(17)

Table **S9** Hydrogen bonds for derivative **A** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(10)-H(10B)...N(8)#1	0.864(19)	2.552(19)	3.2050(16)	133.1(14)
N(10)-H(10B)...N(4)	0.864(19)	2.634(18)	3.2070(15)	124.9(14)
N(10)-H(10A)...N(9)#2	0.903(19)	2.302(19)	3.1629(16)	159.3(15)
N(9)-H(9B)...N(10)#3	0.871(18)	2.581(18)	3.2909(16)	139.2(14)
N(9)-H(9B)...N(7)#4	0.871(18)	2.423(18)	3.1081(15)	135.8(14)
N(9)-H(9A)...N(8)	0.911(18)	2.597(17)	3.1828(15)	122.8(13)
N(9)-H(9A)...N(4)#5	0.911(18)	2.492(18)	3.1653(15)	131.0(14)

Part IV Calculation process of the HOFs for derivative A and B

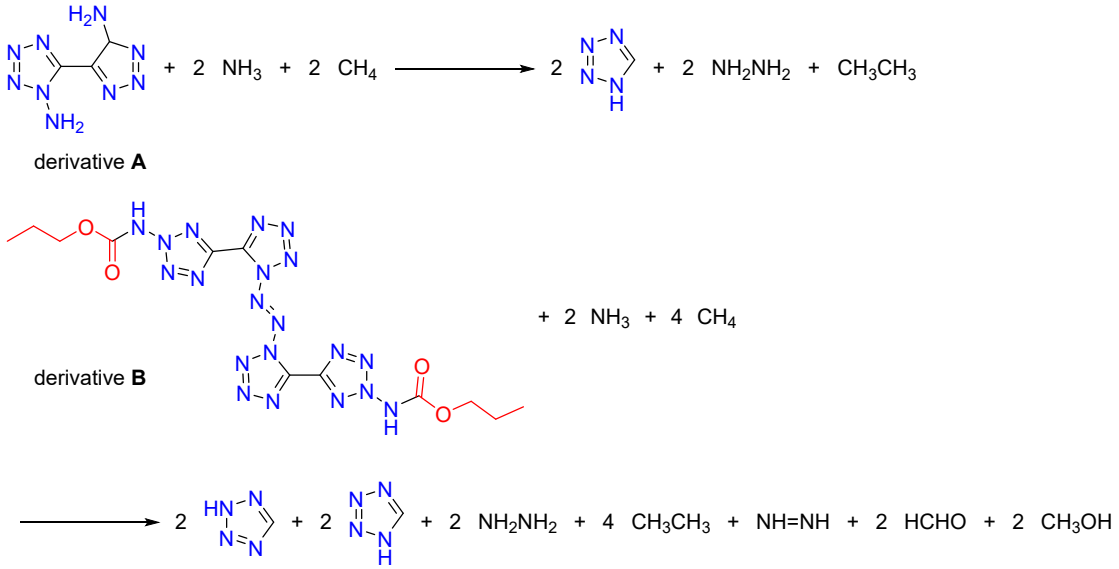

Fig. **S15** Isodesmic reactions of derivative **A** and **B**

Table **S10** Density of derivative **A** and **B** (at M06-2X/6-311g+(2d,p) level)

No.	Volume [a]	Density [b]	overall surface area [c]	$v\sigma_{tot}^2$ [d]	ρ [e]	ΔH_{vap} [f]	ΔH_{sub} [g]	T_{bp} [h]
A	174.4	1.6008	177.5	55.98	1.671	17.50	99.19	662.9
B	536.3	1.5616	498.4	160.5	1.928	41.49	377.0	1714

[a] Angstrom^3; [b] Estimated density according to mass and volume, g/cm^3; [c] Angstrom^2; [d] Product of sigma^2_tot and nu, (kcal/mol)^2; [e] [f] $\Delta H_{vap} = a\sqrt{A} + b\sqrt{v\sigma_{tot}^2} + c$ (kal/mol), $a = 2.130$, $b = 0.930$, $c = -17.844$ (*ref*: *J. Phys. Chem. A.* 2006, **110(3)**, 1005-1013.); [g] $\Delta H_{sub} = aA^2 + b\sqrt{v\sigma_{tot}^2} + c$ (kJ/mol), $a = 0.000267$, $b = 1.650087$, $c = 2.966078$; [h] $T_{bp} = \alpha A + \beta\sqrt{v\sigma_{tot}^2} + \gamma$ (K), $\alpha = 2.736$, $\beta = 33.31$, $\gamma = -72.05$ (*ref*: *J. Phys. Chem.* 1993, **97(37)**, 9369-9373.)

Table **S11** Detonation properties of derivative **A** and **B** (at M06-2X/6-311g+(2d,p) level)

No.	ρ^a	$\Delta H_{f\,b}^0$	OB%[c]	Q^d	D^e	P^f	$h_{50\,g}$
A	1.6008	800.9	38.07	5295	8.170	29.41	47.66
B	1.5616	534.2	-38.08	3333	6.730	19.82	52.90

[a] density (g/cm^3); [b] solid phase heat of formation (kJ/mol); [c] oxygen balance; [d] explosion heat (J/g); [e] detonation velocity (km/s); [f] explosion pressure (GPa); [g] impact sensitivity (cm).