Supporting Information

Enhancing the detonation performance of azobis-triazole energetic derivatives via inducing the *N*-oxide groups

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Detonation performance

For the Kamlet-Jacobs equation, calculations of detonation velocity and detonation pressure can be referenced in the literatures (*The Journal of Chemical Physics*, 1968, 48, 23-35(10.1063/1.1667908); *Central European Journal of Energetic Materials*, 2014, 11(4), 459-474). Among them, four parameters that affect detonation velocity and detonation pressure are determined in the Kamlet-Jacobs equation:

(1) the number of moles N of gaseous detonation products per gram of explosive,

(2) their average molecular mass $\bar{M}$ in g/mol,

(3) the magnitude of the heat release Q for the detonation reaction, in calories per gram of explosive,

(4) its loading density ρ in g/cm^3.

$$D = 1.01\left(N\bar{M}^{\frac{1}{2}}Q^{\frac{1}{2}}\right)^{\frac{1}{2}}(1 + 1.30\rho)$$

$$P = 1.558\rho^2 N\bar{M}^{\frac{1}{2}}Q^{\frac{1}{2}}$$

For EXPLO5, which can predict detonation (e.g. detonation velocity, pressure, energy, heat end temperature, etc.) and combustion (e.g. specific impulse, force, pressure, etc.) performance of energetic materials, is based on the chemical equilibrium steady-state model of detonation. The equilibrium composition of detonation and combustion products is calculated by applying modified White, Johnson, and Dantzig's free energy minimisation technique. The program uses the Becker-Kistiakowsky-Wilson (BKW) and exponential-6 equation of state (Exp-6 EOS) for gaseous detonation products, the ideal gas and virial equations of state of gaseous combustion products, and the Murnaghan equation of states for condensed products. EXPLO5 is designed so that enables calculation of chemical equilibrium composition and thermodynamic parameters of state along the shock adiabat of detonation products, the Chapman-Jouguet (C-J) state and the detonation parameters at the C-J state, as well as the parameters of state along the expansion isentrope. The program has non-linear curve fitting program built in to fit relative volume-pressure data along the expansion isentrope according to the Jones-Wilkins-Lee (JWL) model, enabling the calculation of the detonation energy available for performing mechanical work.

Table S1. Optimized azobis-triazole compounds (**A1** to **F1**) at computational levels with different functionals and different basis sets.

A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.367	N8-C9	1.367
	C2-N3	1.367	N3-N6	1.370
	N3-N13	1.372	N7-N8	1.370
	N13-N14	1.295	N6-N7	1.248
B3LYP/6-31G(d)	N4-C1	1.376	C1-H4	1.079
	C9-C10	1.367	C2-H5	1.077
	C10-N16	1.367	C9-H11	1.077
	N16-N15	1.295	C10-H12	1.079
	N15-N8	1.372		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.367	N8-C9	1.367
	C2-N3	1.367	N3-N6	1.370
	N3-N13	1.372	N7-N8	1.370
	N13-N14	1.295	N6-N7	1.248
B3LYP/6-31G(d,p)	N4-C1	1.376	C1-H4	1.079
	C9-C10	1.367	C2-H5	1.078
	C10-N16	1.367	C9-H11	1.078
	N16-N15	1.295	C10-H12	1.079
	N15-N8	1.372		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.364	N8-C9	1.366
	C2-N3	1.366	N3-N6	1.369
	N3-N13	1.369	N7-N8	1.369
	N13-N14	1.290	N6-N7	1.241
B3LYP/6-311G(d,p)	N4-C1	1.374	C1-H4	1.077
	C9-C10	1.364	C2-H5	1.076
	C10-N16	1.374	C9-H11	1.076
	N16-N15	1.290	C10-H12	1.077
	N15-N8	1.369		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.367	N8-C9	1.367
	C2-N3	1.367	N3-N6	1.370
	N3-N13	1.372	N7-N8	1.370
B3LYP/def2-TZVP	N13-N14	1.291	N6-N7	1.248
	N4-C1	1.374	C1-H4	1.079
	C9-C10	1.376	C2-H5	1.078
	C10-N16	1.376	C9-H11	1.078

	N16-N15	1.291	C10-H12	1.079
	N15-N8	1.372		
B1	Bond	Length (Å)	Bond	Length (Å)
	C1-N2	1.380	N15-C7	1.302
	N2-C13	1.386	C1-H3	1.080
	C13-N9	1.302	C13-H14	1.078
	N9-N16	1.399	C11-H12	1.080
B3LYP/6-31G(d)	N16-C1	1.301	C7-H8	1.078
	C7-N6	1.386	N5-N6	1.368
	N6-C11	1.380	N2-N4	1.368
	C11-N10	1.301	N4-N5	1.252
	N10-N15	1.399		
B1	Bond	Length (Å)	Bond	Length (Å)
	C1-N2	1.380	N15-C7	1.303
	N2-C13	1.386	C1-H3	1.080
	C13-N9	1.303	C13-H14	1.078
	N9-N16	1.398	C11-H12	1.080
B3LYP/6-31G(d,p)	N16-C1	1.301	C7-H8	1.078
	C7-N6	1.386	N5-N6	1.368
	N6-C11	1.380	N2-N4	1.368
	C11-N10	1.301	N4-N5	1.252
	N10-N15	1.398		
B1	Bond	Length (Å)	Bond	Length (Å)
	C1-N2	1.500	N15-C7	2.000
	N2-C13	1.000	C1-H3	1.000
	C13-N9	2.000	C13-H14	1.000
	N9-N16	1.000	C11-H12	1.000
B3LYP/6-311G(d,p)	N16-C1	2.000	C7-H8	1.000
	C7-N6	1.000	N5-N6	1.000
	N6-C11	1.500	N2-N4	1.000
	C11-N10	2.000	N4-N5	2.000
	N10-N15	1.000		
B1	Bond	Length (Å)	Bond	Length (Å)
	C1-N2	1.376	N15-C7	1.296
	N2-C13	1.382	C1-H3	1.077
	C13-N9	1.296	C13-H14	1.075
	N9-N16	1.393	C11-H12	1.077
B3LYP/def2-TZVP	N16-C1	1.294	C7-H8	1.075
	C7-N6	1.382	N5-N6	1.363
	N6-C11	1.376	N2-N4	1.363
	C11-N10	1.294	N4-N5	1.240
	N10-N15	1.393		
C1	Bond	Length (Å)	Bond	Length (Å)

	C3-N13	1.364	C7-C4	1.392
	N13-N5	1.336	C11-H12	1.079
	N5-N10	1.318	N13-H14	1.012
	N10-C11	1.353	N15-H16	1.012
B3LYP/6-31G(d)	C11-C3	1.392	C7-H8	1.079
	C4-N15	1.364	C3-N2	1.380
	N15-N6	1.336	N2-N1	1.380
	N6-N9	1.318	N1-N2	1.272
	N9-C7	1.353		
C1	Bond	Length (Å)	Bond	Length (Å)
	C3-N13	1.364	C7-C4	1.392
	N13-N5	1.337	C11-H12	1.078
	N5-N10	1.318	N13-H14	1.011
	N10-C11	1.353	N15-H16	1.011
B3LYP/6-31G(d,p)	C11-C3	1.392	C7-H8	1.078
	C4-N15	1.364	C3-N2	1.380
	N15-N6	1.337	N2-N1	1.380
	N6-N9	1.318	N1-N2	1.272
	N9-C7	1.353		
C1	Bond	Length (Å)	Bond	Length (Å)
	C3-N13	1.362	C7-C4	1.389
	N13-N5	1.334	C11-H12	1.076
	N5-N10	1.314	N13-H14	1.010
	N10-C11	1.351	N15-H16	1.010
B3LYP/6-311G(d,p)	C11-C3	1.389	C7-H8	1.076
	C4-N15	1.363	C3-N1	1.378
	N15-N6	1.334	N2-C4	1.378
	N6-N9	1.314	N1-N2	1.266
	N9-C7	1.351		
C1	Bond	Length (Å)	Bond	Length (Å)
	C3-N13	1.359	C7-C4	1.387
	N13-N5	1.329	C11-H12	1.075
	N5-N10	1.311	N13-H14	1.009
	N10-C11	1.348	N15-H16	1.009
B3LYP/def2-TZVP	C11-C3	1.387	C7-H8	1.075
	C4-N15	1.359	C3-N1	1.376
	N15-N6	1.329	N2-C4	1.376
	N6-N9	1.311	N1-N2	1.260
	N9-C7	1.348		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.374	N7-C15	1.325
	N10-C13	1.356	C11-H12	1.080
B3LYP/6-31G(d)	C13-N6	1.322	N9-H4	1.011
	N6-N5	1.368	C13-H14	1.080

	N5-C16	1.325	N10-H1	1.011
	C15-N9	1.374	C16-N2	1.386
	N9-C11	1.356	C15-N3	1.386
	C11-N8	1.322	N2-N3	1.266
	N8-N7	1.368		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.373	N7-C15	1.325
	N10-C13	1.356	C11-H12	1.080
	C13-N6	1.322	N9-H4	1.010
	N6-N5	1.367	C13-H14	1.080
B3LYP/6-31G(d,p)	N5-C16	1.325	N10-H1	1.010
	C15-N9	1.373	C16-N2	1.386
	N9-C11	1.356	C15-N3	1.386
	C11-N8	1.322	N2-N3	1.266
	N8-N7	1.367		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.372	N7-C15	1.320
	N10-C13	1.355	C11-H12	1.078
	C13-N6	1.318	N9-H4	1.009
	N6-N5	1.365	C13-H14	1.078
B3LYP/6-311G(d,p)	N5-C16	1.320	N10-H1	1.009
	C15-N9	1.372	C16-N2	1.384
	N9-C11	1.355	C15-N3	1.384
	C11-N8	1.318	N2-N3	1.260
	N8-N7	1.365		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.369	N7-C15	1.317
	N10-C13	1.351	C11-H12	1.077
	C13-N6	1.316	N9-H4	1.077
	N6-N5	1.362	C13-H14	1.077
B3LYP/def2-TZVP	N5-C16	1.317	N10-H1	1.077
	C15-N9	1.369	C16-N2	1.382
	N9-C11	1.351	C15-N3	1.382
	C11-N8	1.316	N2-N3	1.254
	N8-N7	1.362		
E1	Bond	Length (Å)	Bond	Length (Å)
	N6-N16	1.342	N9-N2	1.344
	N16-C7	1.326	C13-H14	1.081
	C7-C13	1.417	C7-H8	1.080
	C13-N10	1.327	C11-H12	1.081
B3LYP/6-31G(d)	N10-N6	1.344	C1-H3	1.080
	N2-N15	1.342	N4-N2	1.370
	N15-C1	1.326	N5-N6	1.370
	C1-C11	1.417	N4-N5	1.249

	C11-N9	1.327		
E1	Bond	Length (Å)	Bond	Length (Å)
B3LYP/6-31G(d,p)	N6-N16	1.342	N9-N2	1.344
	N16-C7	1.326	C13-H14	1.080
	C7-C13	1.416	C7-H8	1.080
	C13-N10	1.327	C11-H12	1.080
	N10-N6	1.344	C1-H3	1.080
	N2-N15	1.342	N4-N2	1.370
	N15-C1	1.326	N5-N6	1.370
	C1-C11	1.416	N4-N5	1.249
	C11-N9	1.327		
E1	Bond	Length (Å)	Bond	Length (Å)
B3LYP/6-311G(d,p)	N6-N16	1.339	N9-N2	1.341
	N16-C7	1.322	C13-H14	1.079
	C7-C13	1.416	C7-H8	1.078
	C13-N10	1.323	C11-H12	1.079
	N10-N6	1.341	C1-H3	1.078
	N2-N15	1.339	N4-N2	1.368
	N15-C1	1.322	N5-N6	1.368
	C1-C11	1.416	N4-N5	1.242
	C11-N9	1.323		
E1	Bond	Length (Å)	Bond	Length (Å)
B3LYP/def2-TZVP	N6-N16	1.335	N9-N2	1.336
	N16-C7	1.320	C13-H14	1.077
	C7-C13	1.412	C7-H8	1.077
	C13-N10	1.321	C11-H12	1.077
	N10-N6	1.336	C1-H3	1.077
	N2-N15	1.335	N4-N2	1.364
	N15-C1	1.320	N5-N6	1.364
	C1-C11	1.412	N4-N5	1.238
	C11-N9	1.321		
F1	Bond	Length (Å)	Bond	Length (Å)
B3LYP/6-31G(d)	N4-C13	1.367	N5-N1	1.364
	C13-N16	1.311	C9-H10	1.082
	N16-C9	1.374	C13-H14	1.081
	C9-N6	1.320	C7-H8	1.082
	N6-N4	1.364	C11-H12	1.081
	N1-C11	1.367	N4-N3	1.366
	C11-N15	1.311	N1-N2	1.366
	N15-C7	1.374	N2-N3	1.249
	C7-N5	1.320		
F1	Bond	Length (Å)	Bond	Length (Å)
B3LYP/6-31G(d,p)	N4-C13	1.367	N5-N1	1.363

	C13-N16	1.312	C9-H10	1.081
	N16-C9	1.374	C13-H14	1.080
	C9-N6	1.321	C7-H8	1.081
	N6-N4	1.363	C11-H12	1.080
	N1-C11	1.367	N4-N3	1.366
	C11-N15	1.312	N1-N2	1.366
	N15-C7	1.374	N2-N3	1.249
	C7-N5	1.321		
F1	Bond	Length (Å)	Bond	Length (Å)
	N4-C13	1.367	N5-N1	1.360
	C13-N16	1.308	C9-H10	1.079
	N16-C9	1.373	C13-H14	1.078
	C9-N6	1.317	C7-H8	1.079
B3LYP/6-311G(d,p)	N6-N4	1.360	C11-H12	1.078
	N1-C11	1.367	N4-N3	1.364
	C11-N15	1.308	N1-N2	1.364
	N15-C7	1.373	N2-N3	1.242
	C7-N5	1.317		
F1	Bond	Length (Å)	Bond	Length (Å)
	N4-C13	1.362	N5-N1	1.357
	C13-N16	1.306	C9-H10	1.078
	N16-C9	1.369	C13-H14	1.077
	C9-N6	1.314	C7-H8	1.078
B3LYP/def2-TZVP	N6-N4	1.357	C11-H12	1.077
	N1-C11	1.362	N4-N3	1.361
	C11-N15	1.306	N1-N2	1.361
	N15-C7	1.369	N2-N3	1.238
	C7-N5	1.314		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.360	N8-C9	1.357
	C2-N3	1.357	N3-N6	1.365
	N3-N13	1.344	N7-N8	1.365
	N13-N14	1.281	N6-N7	1.226
M06-2X/631G(d)	N4-C1	1.368	C1-H4	1.075
	C9-C10	1.360	C2-H5	1.075
	C10-N16	1.368	C9-H11	1.075
	N16-N15	1.281	C10-H12	1.075
	N15-N8	1.344		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.364	N8-C9	1.361
	C2-N3	1.361	N3-N6	1.368
M06-2X/6-31G(d,p)	N3-N13	1.351	N7-N8	1.368
	N13-N14	1.285	N6-N7	1.235
	N14-C1	1.371	C1-H4	1.078

	C9-C10	1.364	C2-H5	1.078
	C10-N16	1.371	C9-H11	1.078
	N16-N15	1.285	C10-H12	1.078
	N15-N8	1.351		
A1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-311G(d,p)	C1-C2	1.364	N8-C9	1.361
	C2-N3	1.361	N3-N6	1.368
	N3-N13	1.351	N7-N8	1.368
	N13-N14	1.285	N6-N7	1.235
	N14-C1	1.372	C1-H4	1.078
	C9-C10	1.364	C2-H5	1.077
	C10-N16	1.372	C9-H11	1.077
	N16-N15	1.285	C10-H12	1.078
	N15-N8	1.351		
A1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/def2-TZVP	C1-C2	1.362	N8-C9	1.360
	C2-N3	1.360	N3-N6	1.367
	N3-N13	1.349	N7-N8	1.367
	N13-N14	1.282	N6-N7	1.229
	N14-C1	1.371	C1-H4	1.076
	C9-C10	1.362	C2-H5	1.076
	C10-N16	1.371	C9-H11	1.076
	N16-N15	1.282	C10-H12	1.076
	N15-N8	1.349		
B1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-31G(d)	C1-N2	1.370	N15-C7	1.292
	N2-C13	1.376	C1-H3	1.077
	C13-N9	1.292	C13-H14	1.076
	N9-N16	1.381	C11-H12	1.077
	N16-C1	1.291	C7-H8	1.076
	C7-N6	1.376	N5-N6	1.360
	N6-C11	1.370	N2-N4	1.360
	C11-N10	1.291	N4-N5	1.229
	N10-N15	1.381		
B1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-31G(d,p)	C1-N2	1.374	N15-C7	1.297
	N2-C13	1.379	C1-H3	1.080
	C13-N9	1.297	C13-H14	1.079
	N9-N16	1.384	C11-H12	1.080
	N16-C1	1.296	C7-H8	1.079
	C7-N6	1.379	N5-N6	1.363
	N6-C11	1.374	N2-N4	1.363
	C11-N10	1.296	N4-N5	1.239

	N10-N15	1.384		
B1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-311G(d,p)	C1-N2	1.373	N15-C7	1.298
	N2-C13	1.379	C1-H3	1.079
	C13-N9	1.298	C13-H14	1.078
	N9-N16	1.383	C11-H12	1.079
	N16-C1	1.296	C7-H8	1.078
	C7-N6	1.379	N5-N6	1.363
	N6-C11	1.373	N2-N4	1.363
	C11-N10	1.296	N4-N5	1.239
	N10-N15	1.383		
B1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/def2-TZVP	C1-N2	1.374	N15-C7	1.294
	N2-C13	1.380	C1-H3	1.078
	C13-N9	1.294	C13-H14	1.076
	N9-N16	1.384	C11-H12	1.078
	N16-C1	1.292	C7-H8	1.076
	C7-N6	1.380	N5-N6	1.362
	N6-C11	1.374	N2-N4	1.362
	C11-N10	1.292	N4-N5	1.233
	N10-N15	1.384		
C1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-31G(d)	C3-N13	1.352	C7-C4	1.378
	N13-N5	1.320	C11-H12	1.075
	N5-N10	1.300	N13-H14	1.009
	N10-C11	1.349	N15-H16	1.009
	C11-C3	1.378	C7-H8	1.075
	C4-N15	1.352	C3-N1	1.386
	N15-N6	1.320	N2-C4	1.386
	N6-N9	1.300	N1-N2	1.244
	N9-C7	1.349		
C1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-31G(d,p)	C3-N13	1.356	C7-C4	1.383
	N13-N5	1.325	C11-H12	1.078
	N5-N10	1.305	N13-H14	1.012
	N10-C11	1.352	N15-H16	1.012
	C11-C3	1.383	C7-H8	1.078
	C4-N15	1.356	C3-N1	1.388
	N15-N6	1.325	N2-N4	1.388
	N6-N9	1.305	N1-N2	1.254
	N9-C7	1.352		
C1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-311G(d,p)	C3-N13	1.355	C7-C4	1.382

	N13-N5	1.326	C11-H12	1.078
	N5-N10	1.304	N13-H14	1.010
	N10-C11	1.352	N15-H16	1.010
	C11-C3	1.382	C7-H8	1.078
	C4-N15	1.355	C3-N1	1.388
	N15-N6	1.326	N2-C4	1.388
	N6-N9	1.304	N1-N2	1.254
	N9-C7	1.352		
C1	Bond	Length (Å)	Bond	Length (Å)
	C3-N13	1.355	C7-C4	1.380
	N13-N5	1.324	C11-H12	1.076
	N5-N10	1.301	N13-H14	1.010
	N10-C11	1.351	N15-H16	1.010
M06-2X/def2-TZVP	C11-C3	1.380	C7-H8	1.076
	C4-N15	1.355	C3-N1	1.387
	N15-N6	1.324	N2-C4	1.387
	N6-N9	1.301	N1-N2	1.249
	N9-C7	1.351		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.361	N7-C15	1.307
	N10-C13	1.350	C11-H12	1.077
	C13-N6	1.309	N9-H4	1.007
	N6-N5	1.357	C13-H14	1.077
M06-2X/6-31G(d)	N5-C16	1.307	N10-H1	1.007
	C15-N9	1.361	C16-N2	1.394
	N9-C11	1.350	C15-N3	1.394
	C11-N8	1.309	N2-N3	1.238
	N8-N7	1.357		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.365	N7-C15	1.313
	N10-C13	1.353	C11-H12	1.080
	C13-N6	1.315	N9-H4	1.011
	N6-N5	1.359	C13-H14	1.080
M06-2X/6-31G(d,p)	N5-C16	1.313	N10-H1	1.011
	C15-N9	1.365	C16-N2	1.395
	N9-C11	1.353	C15-N3	1.395
	C11-N8	1.315	N2-N3	1.249
	N8-N7	1.359		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.364	N7-C15	1.313
	N10-C13	1.353	C11-H12	1.079
M06-2X/6-311G(d,p)	C13-N6	1.315	N9-H4	1.009
	N6-N5	1.359	C13-H14	1.079
	N5-C16	1.313	N10-H1	1.009

	C15-N9	1.364	C16-N2	1.396
	N9-C11	1.353	C15-N3	1.396
	C11-N8	1.315	N2-N3	1.249
	N8-N7	1.359		
D1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/def2-TZVP	C16-N10	1.364	N7-C15	1.309
	N10-C13	1.353	C11-H12	1.077
	C13-N6	1.311	N9-H4	1.009
	N6-N5	1.358	C13-H14	1.077
	N5-C16	1.309	N10-H1	1.009
	C15-N9	1.364	C16-N2	1.394
	N9-C11	1.353	C15-N3	1.394
	C11-N8	1.311	N2-N3	1.243
	N8-N7	1.358		
E1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-31G(d)	N6-N16	1.323	N9-N2	1.323
	N16-C7	1.316	C13-H14	1.077
	C7-C13	1.411	C7-H8	1.076
	C13-N10	1.317	C11-H12	1.077
	N10-N6	1.323	C1-H3	1.076
	N2-N15	1.323	N4-N2	1.365
	N15-C1	1.316	N5-N6	1.365
	C1-C11	1.411	N4-N5	1.226
	C11-N9	1.317		
E1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-31G(d,p)	N6-N16	1.328	N9-N2	1.329
	N16-C7	1.320	C13-H14	1.080
	C7-C13	1.415	C7-H8	1.079
	C13-N10	1.321	C11-H12	1.080
	N10-N6	1.329	C1-H3	1.079
	N2-N15	1.328	N4-N2	1.368
	N15-C1	1.320	N5-N6	1.368
	C1-C11	1.415	N4-N5	1.235
	C11-N9	1.321		
E1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-311G(d,p)	N6-N16	1.328	N9-N2	1.329
	N16-C7	1.320	C13-H14	1.079
	C7-C13	1.415	C7-H8	1.079
	C13-N10	1.321	C11-H12	1.079
	N10-N6	1.329	C1-H3	1.079
	N2-N15	1.328	N4-N2	1.368
	N15-C1	1.320	N5-N6	1.368
	C1-C11	1.415	N4-N5	1.235

	C11-N9	1.321		
E1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/def2-TZVP	N6-N16	1.326	N9-N2	1.328
	N16-C7	1.317	C13-H14	1.078
	C7-C13	1.414	C7-H8	1.077
	C13-N10	1.318	C11-H12	1.078
	N10-N6	1.328	C1-H3	1.077
	N2-N15	1.326	N4-N2	1.368
	N15-C1	1.317	N5-N6	1.368
	C1-C11	1.414	N4-N5	1.230
	C11-N9	1.318		
F1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-31G(d)	N4-C13	1.355	N5-N1	1.345
	C13-N16	1.303	C9-H10	1.078
	N16-C9	1.367	C13-H14	1.078
	C9-N6	1.310	C7-H8	1.078
	N6-N4	1.345	C11-H12	1.078
	N1-C11	1.355	N4-N3	1.360
	C11-N15	1.303	N1-N2	1.360
	N15-C7	1.367	N2-N3	1.227
	C7-N5	1.310		
F1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-31G(d,p)	N4-C13	1.359	N5-N1	1.349
	C13-N16	1.306	C9-H10	1.081
	N16-C9	1.370	C13-H14	1.081
	C9-N6	1.315	C7-H8	1.081
	N6-N4	1.349	C11-H12	1.081
	N1-C11	1.359	N4-N3	1.363
	C11-N15	1.306	N1-N2	1.363
	N15-C7	1.370	N2-N3	1.236
	C7-N5	1.315		
F1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/6-311G(d,p)	N4-C13	1.359	N5-N1	1.349
	C13-N16	1.307	C9-H10	1.080
	N16-C9	1.370	C13-H14	1.080
	C9-N6	1.315	C7-H8	1.080
	N6-N4	1.349	C11-H12	1.080
	N1-C11	1.359	N4-N3	1.363
	C11-N15	1.307	N1-N2	1.363
	N15-C7	1.370	N2-N3	1.236
	C7-N5	1.315		
F1	Bond	Length (Å)	Bond	Length (Å)
M06-2X/def2-TZVP	N4-C13	1.359	N5-N1	1.348

	C13-N16	1.304	C9-H10	1.079
	N16-C9	1.369	C13-H14	1.079
	C9-N6	1.312	C7-H8	1.079
	N6-N4	1.348	C11-H12	1.079
	N1-C11	1.359	N4-N3	1.362
	C11-N15	1.304	N1-N2	1.362
	N15-C7	1.369	N2-N3	1.230
	C7-N5	1.312		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.359	N8-C9	1.357
	C2-N3	1.357	N3-N6	1.356
	N3-N13	1.347	N7-N8	1.356
	N13-N14	1.283	N6-N7	1.232
PBE0/6-31G(d)	N4-C1	1.365	C1-H4	1.077
	C9-C10	1.359	C2-H5	1.076
	C10-N16	1.365	C9-H11	1.076
	N16-N15	1.283	C10-H12	1.077
	N15-N8	1.347		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.364	N8-C9	1.361
	C2-N3	1.361	N3-N6	1.360
	N3-N13	1.354	N7-N8	1.360
	N13-N14	1.288	N6-N7	1.241
PBE0/6-31G(d,p)	N14-C1	1.369	C1-H4	1.080
	C9-C10	1.364	C2-H5	1.078
	C10-N16	1.369	C9-H11	1.078
	N16-N15	1.288	C10-H12	1.080
	N15-N8	1.354		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.364	N8-C9	1.361
	C2-N3	1.361	N3-N6	1.360
	N3-N13	1.354	N7-N8	1.360
	N13-N14	1.288	N6-N7	1.241
PBE0/6-311G(d,p)	N14-C1	1.369	C1-H4	1.079
	C9-C10	1.364	C2-H5	1.078
	C10-N16	1.369	C9-H11	1.078
	N16-N15	1.288	C10-H12	1.079
	N15-N8	1.354		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.362	N8-C9	1.360
	C2-N3	1.360	N3-N6	1.358
PBE0/def2-TZVP	N3-N13	1.352	N7-N8	1.358
	N13-N14	1.283	N6-N7	1.235
	N14-C1	1.367	C1-H4	1.078

	C9-C10	1.362	C2-H5	1.077
	C10-N16	1.367	C9-H11	1.077
	N16-N15	1.283	C10-H12	1.078
	N15-N8	1.352		
B1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-31G(d)	C1-N2	1.369	N15-C7	1.294
	N2-C13	1.374	C1-H3	1.079
	C13-N9	1.294	C13-H14	1.077
	N9-N16	1.378	C11-H12	1.079
	N16-C1	1.292	C7-H8	1.077
	C7-N6	1.374	N5-N6	1.353
	N6-C11	1.369	N2-N4	1.353
	C11-N10	1.292	N4-N5	1.235
	N10-N15	1.378		
B1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-31G(d,p)	C1-N2	1.373	N15-C7	1.299
	N2-C13	1.377	C1-H3	1.080
	C13-N9	1.299	C13-H14	1.079
	N9-N16	1.383	C11-H12	1.080
	N16-C1	1.297	C7-H8	1.079
	C7-N6	1.377	N5-N6	1.357
	N6-C11	1.373	N2-N4	1.357
	C11-N10	1.297	N4-N5	1.245
	N10-N15	1.383		
B1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-311G(d,p)	C1-N2	1.373	N15-C7	1.299
	N2-C13	1.377	C1-H3	1.080
	C13-N9	1.299	C13-H14	1.078
	N9-N16	1.382	C11-H12	1.080
	N16-C1	1.298	C7-H8	1.078
	C7-N6	1.377	N5-N6	1.357
	N6-C11	1.373	N2-N4	1.357
	C11-N10	1.298	N4-N5	1.245
	N10-N15	1.382		
B1	Bond	Length (Å)	Bond	Length (Å)
PBE0/def2-TZVP	C1-N2	1.372	N15-C7	1.295
	N2-C13	1.377	C1-H3	1.079
	C13-N9	1.295	C13-H14	1.077
	N9-N16	1.381	C11-H12	1.079
	N16-C1	1.294	C7-H8	1.077
	C7-N6	1.377	N5-N6	1.355
	N6-C11	1.372	N2-N4	1.355
	C11-N10	1.294	N4-N5	1.238

	N10-N15	1.381		
C1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-31G(d)	C3-N13	1.353	C7-C4	1.383
	N13-N5	1.318	C11-H12	1.077
	N5-N10	1.303	N13-H14	1.008
	N10-C11	1.344	N15-H16	1.008
	C11-C3	1.383	C7-H8	1.077
	C4-N15	1.353	C3-N2	1.373
	N15-N6	1.318	N2-N1	1.373
	N6-N9	1.303	N1-N2	1.253
	N9-C7	1.344		
C1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-31G(d,p)	C3-N13	1.357	C7-C4	1.387
	N13-N5	1.324	C11-H12	1.079
	N5-N10	1.309	N13-H14	1.011
	N10-C11	1.347	N15-H16	1.011
	C11-C3	1.387	C7-H8	1.079
	C4-N15	1.357	C3-N1	1.376
	N15-N6	1.324	N2-N4	1.376
	N6-N9	1.309	N1-N2	1.263
	N9-C7	1.347		
C1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-311G(d,p)	C3-N13	1.357	C7-C4	1.387
	N13-N5	1.325	C11-H12	1.079
	N5-N10	1.309	N13-H14	1.010
	N10-C11	1.348	N15-H16	1.010
	C11-C3	1.387	C7-H8	1.079
	C4-N15	1.357	C3-N1	1.376
	N15-N6	1.325	N2-C4	1.376
	N6-N9	1.309	N1-N2	1.263
	N9-C7	1.348		
C1	Bond	Length (Å)	Bond	Length (Å)
PBE0/def2-TZVP	C3-N13	1.356	C7-C4	1.385
	N13-N5	1.321	C11-H12	1.077
	N5-N10	1.305	N13-H14	1.009
	N10-C11	1.346	N15-H16	1.009
	C11-C3	1.385	C7-H8	1.077
	C4-N15	1.356	C3-N1	1.374
	N15-N6	1.321	N2-C4	1.374
	N6-N9	1.305	N1-N2	1.257
	N9-C7	1.346		
D1	Bond	Length	Bond	Length
PBE0/6-31G(d)	Bond	Length (Å)	Bond	Length (Å)

	N10-C13	1.345	C11-H12	1.079
	C13-N6	1.313	N9-H4	1.007
	N6-N5	1.350	C13-H14	1.079
	N5-C16	1.314	N10-H1	1.007
	C15-N9	1.361	C16-N2	1.378
	N9-C11	1.345	C15-N3	1.378
	C11-N8	1.313	N2-N3	1.248
	N8-N7	1.350		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.366	N7-C15	1.320
	N10-C13	1.349	C11-H12	1.081
	C13-N6	1.318	N9-H4	1.010
	N6-N5	1.354	C13-H14	1.081
PBE0/6-31G(d,p)	N5-C16	1.320	N10-H1	1.010
	C15-N9	1.366	C16-N2	1.381
	N9-C11	1.349	C15-N3	1.381
	C11-N8	1.318	N2-N3	1.258
	N8-N7	1.354		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.365	N7-C15	1.320
	N10-C13	1.349	C11-H12	1.080
	C13-N6	1.318	N9-H4	1.008
	N6-N5	1.354	C13-H14	1.080
PBE0/6-311G(d,p)	N5-C16	1.320	N10-H1	1.008
	C15-N9	1.365	C16-N2	1.381
	N9-C11	1.349	C15-N3	1.381
	C11-N8	1.318	N2-N3	1.258
	N8-N7	1.354		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.364	N7-C15	1.315
	N10-C13	1.348	C11-H12	1.079
	C13-N6	1.315	N9-H4	1.008
	N6-N5	1.352	C13-H14	1.079
PBE0/def2-TZVP	N5-C16	1.315	N10-H1	1.008
	C15-N9	1.364	C16-N2	1.379
	N9-C11	1.348	C15-N3	1.379
	C11-N8	1.315	N2-N3	1.252
	N8-N7	1.352		
E1	Bond	Length (Å)	Bond	Length (Å)
	N6-N16	1.324	N9-N2	1.324
	N16-C7	1.317	C13-H14	1.079
PBE0/6-31G(d)	C7-C13	1.408	C7-H8	1.078
	C13-N10	1.318	C11-H12	1.079
	N10-N6	1.324	C1-H3	1.078

	N2-N15	1.324	N4-N2	1.355
	N15-C1	1.317	N5-N6	1.355
	C1-C11	1.408	N4-N5	1.233
	C11-N9	1.318		
E1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-31G(d,p)	N6-N16	1.330	N9-N2	1.331
	N16-C7	1.321	C13-H14	1.081
	C7-C13	1.412	C7-H8	1.080
	C13-N10	1.322	C11-H12	1.081
	N10-N6	1.331	C1-H3	1.080
	N2-N15	1.330	N4-N2	1.360
	N15-C1	1.321	N5-N6	1.360
	C1-C11	1.412	N4-N5	1.242
	C11-N9	1.322		
E1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-311G(d,p)	N6-N16	1.330	N9-N2	1.331
	N16-C7	1.321	C13-H14	1.080
	C7-C13	1.412	C7-H8	1.080
	C13-N10	1.323	C11-H12	1.080
	N10-N6	1.331	C1-H3	1.080
	N2-N15	1.330	N4-N2	1.360
	N15-C1	1.321	N5-N6	1.360
	C1-C11	1.412	N4-N5	1.242
	C11-N9	1.323		
E1	Bond	Length (Å)	Bond	Length (Å)
PBE0/def2-TZVP	N6-N16	1.327	N9-N2	1.328
	N16-C7	1.318	C13-H14	1.079
	C7-C13	1.411	C7-H8	1.079
	C13-N10	1.319	C11-H12	1.079
	N10-N6	1.328	C1-H3	1.079
	N2-N15	1.327	N4-N2	1.358
	N15-C1	1.318	N5-N6	1.358
	C1-C11	1.411	N4-N5	1.236
	C11-N9	1.319		
F1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-31G(d)	N4-C13	1.355	N5-N1	1.344
	C13-N16	1.303	C9-H10	1.080
	N16-C9	1.363	C13-H14	1.080
	C9-N6	1.311	C7-H8	1.079
	N6-N4	1.344	C11-H12	1.079
	N1-C11	1.355	N4-N3	1.351
	C11-N15	1.303	N1-N2	1.351
	N15-C7	1.363	N2-N3	1.233

	C7-N5	1.311		
F1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-31G(d,p)	N4-C13	1.360	N5-N1	1.350
	C13-N16	1.307	C9-H10	1.082
	N16-C9	1.367	C13-H14	1.081
	C9-N6	1.316	C7-H8	1.082
	N6-N4	1.350	C11-H12	1.081
	N1-C11	1.360	N4-N3	1.355
	C11-N15	1.307	N1-N2	1.355
	N15-C7	1.367	N2-N3	1.242
	C7-N5	1.316		
F1	Bond	Length (Å)	Bond	Length (Å)
PBE0/6-311G(d,p)	N4-C13	1.360	N5-N1	1.349
	C13-N16	1.308	C9-H10	1.081
	N16-C9	1.367	C13-H14	1.081
	C9-N6	1.316	C7-H8	1.081
	N6-N4	1.349	C11-H12	1.081
	N1-C11	1.360	N4-N3	1.355
	C11-N15	1.308	N1-N2	1.355
	N15-C7	1.367	N2-N3	1.242
	C7-N5	1.316		
F1	Bond	Length (Å)	Bond	Length (Å)
PBE0/def2-TZVP	N4-C13	1.359	N5-N1	1.347
	C13-N16	1.305	C9-H10	1.080
	N16-C9	1.366	C13-H14	1.079
	C9-N6	1.313	C7-H8	1.080
	N6-N4	1.347	C11-H12	1.079
	N1-C11	1.359	N4-N3	1.354
	C11-N15	1.305	N1-N2	1.354
	N15-C7	1.366	N2-N3	1.236
	C7-N5	1.313		
A1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-31G(d)	C1-C2	1.358	N8-C9	1.356
	C2-N3	1.356	N3-N6	1.364
	N3-N13	1.348	N7-N8	1.364
	N13-N14	1.282	N6-N7	1.227
	N14-C1	1.366	C1-H4	1.076
	C9-C10	1.358	C2-H5	1.075
	C10-N16	1.366	C9-H11	1.075
	N16-N15	1.282	C10-H12	1.076
	N15-N8	1.348		
A1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-31G(d,p)	C1-C2	1.363	N8-C9	1.361

	C2-N3	1.361	N3-N6	1.368
	N3-N13	1.357	N7-N8	1.368
	N13-N14	1.288	N6-N7	1.238
	N14-C1	1.371	C1-H4	1.079
	C9-C10	1.363	C2-H5	1.078
	C10-N16	1.371	C9-H11	1.078
	N16-N15	1.288	C10-H12	1.079
	N15-N8	1.357		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.363	N8-C9	1.361
	C2-N3	1.361	N3-N6	1.368
	N3-N13	1.356	N7-N8	1.368
	N13-N14	1.288	N6-N7	1.238
ωB97XD/6-311G(d,p)	N14-C1	1.371	C1-H4	1.078
	C9-C10	1.363	C2-H5	1.077
	C10-N16	1.371	C9-H11	1.077
	N16-N15	1.288	C10-H12	1.078
	N15-N8	1.356		
A1	Bond	Length (Å)	Bond	Length (Å)
	C1-C2	1.361	N8-C9	1.360
	C2-N3	1.360	N3-N6	1.366
	N3-N13	1.353	N7-N8	1.366
	N13-N14	1.283	N6-N7	1.231
ωB97XD/def2-TZVP	N14-C1	1.369	C1-H4	1.077
	C9-C10	1.361	C2-H5	1.076
	C10-N16	1.369	C9-H11	1.076
	N16-N15	1.283	C10-H12	1.077
	N15-N8	1.353		
B1	Bond	Length (Å)	Bond	Length (Å)
	C1-N2	1.369	N15-C7	1.292
	N2-C13	1.375	C1-H3	1.077
	C13-N9	1.292	C13-H14	1.076
	N9-N16	1.383	C11-H12	1.077
ωB97XD/6-31G(d)	N16-C1	1.291	C7-H8	1.076
	C7-N6	1.369	N5-N6	1.359
	N6-C11	1.369	N2-N4	1.359
	C11-N10	1.291	N4-N5	1.231
	N10-N15	1.383		
B1	Bond	Length (Å)	Bond	Length (Å)
	C1-N2	1.373	N15-C7	1.298
	N2-C13	1.379	C1-H3	1.080
ωB97XD/6-31G(d,p)	C13-N9	1.298	C13-H14	1.078
	N9-N16	1.388	C11-H12	1.080
	N16-C1	1.297	C7-H8	1.078

	C7-N6	1.373	N5-N6	1.364
	N6-C11	1.373	N2-N4	1.364
	C11-N10	1.297	N4-N5	1.242
	N10-N15	1.388		
B1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-311G(d,p)	C1-N2	1.373	N15-C7	1.298
	N2-C13	1.379	C1-H3	1.079
	C13-N9	1.298	C13-H14	1.078
	N9-N16	1.387	C11-H12	1.079
	N16-C1	1.297	C7-H8	1.078
	C7-N6	1.379	N5-N6	1.364
	N6-C11	1.373	N2-N4	1.364
	C11-N10	1.297	N4-N5	1.241
	N10-N15	1.387		
B1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/def2-TZVP	C1-N2	1.373	N15-C7	1.294
	N2-C13	1.379	C1-H3	1.078
	C13-N9	1.294	C13-H14	1.077
	N9-N16	1.386	C11-H12	1.078
	N16-C1	1.292	C7-H8	1.077
	C7-N6	1.373	N5-N6	1.362
	N6-C11	1.373	N2-N4	1.362
	C11-N10	1.292	N4-N5	1.235
	N10-N15	1.386		
C1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-31G(d)	C3-N13	1.351	C7-C4	1.377
	N13-N5	1.321	C11-H12	1.075
	N5-N10	1.301	N13-H14	1.007
	N10-C11	1.348	N15-H16	1.007
	C11-C3	1.377	C7-H8	1.075
	C4-N15	1.377	C3-N1	1.383
	N15-N6	1.321	N2-C4	1.383
	N6-N9	1.301	N1-N2	1.246
	N9-C7	1.348		
C1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-31G(d,p)	C3-N13	1.356	C7-C4	1.382
	N13-N5	1.329	C11-H12	1.078
	N5-N10	1.308	N13-H14	1.010
	N10-C11	1.352	N15-H16	1.010
	C11-C3	1.382	C7-H8	1.078
	C4-N15	1.356	C3-N1	1.386
	N15-N6	1.329	N2-C4	1.386
	N6-N9	1.308	N1-N2	1.257

	N9-C7	1.352		
C1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-311G(d,p)	C3-N13	1.356	C7-C4	1.382
	N13-N5	1.330	C11-H12	1.078
	N5-N10	1.307	N13-H14	1.009
	N10-C11	1.352	N15-H16	1.009
	C11-C3	1.382	C7-H8	1.078
	C4-N15	1.356	C3-N1	1.386
	N15-N6	1.330	N2-C4	1.386
	N6-N9	1.307	N1-N2	1.257
	N9-C7	1.352		
C1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/def2-TZVP	C3-N13	1.355	C7-C4	1.379
	N13-N5	1.326	C11-H12	1.076
	N5-N10	1.303	N13-H14	1.008
	N10-C11	1.350	N15-H16	1.008
	C11-C3	1.379	C7-H8	1.076
	C4-N15	1.355	C3-N1	1.385
	N15-N6	1.326	N2-C4	1.385
	N6-N9	1.303	N1-N2	1.251
	N9-C7	1.350		
D1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-31G(d)	C16-N10	1.360	N7-C15	1.307
	N10-C13	1.349	C11-H12	1.077
	C13-N6	1.309	N9-H4	1.005
	N6-N5	1.358	C13-H14	1.077
	N5-C16	1.307	N10-H1	1.005
	C15-N9	1.360	C16-N2	1.390
	N9-C11	1.349	C15-N3	1.390
	C11-N8	1.309	N2-N3	1.240
	N8-N7	1.358		
D1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-31G(d,p)	C16-N10	1.365	N7-C15	1.315
	N10-C13	1.353	C11-H12	1.080
	C13-N6	1.315	N9-H4	1.009
	N6-N5	1.363	C13-H14	1.080
	N5-C16	1.315	N10-H1	1.009
	C15-N9	1.365	C16-N2	1.393
	N9-C11	1.353	C15-N3	1.393
	C11-N8	1.315	N2-N3	1.252
	N8-N7	1.363		
D1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-311G(d,p)	C16-N10	1.365	N7-C15	1.314

	N10-C13	1.353	C11-H12	1.079
	C13-N6	1.315	N9-H4	1.008
	N6-N5	1.363	C13-H14	1.079
	N5-C16	1.314	N10-H1	1.008
	C15-N9	1.365	C16-N2	1.393
	N9-C11	1.353	C15-N3	1.393
	C11-N8	1.315	N2-N3	1.252
	N8-N7	1.363		
D1	Bond	Length (Å)	Bond	Length (Å)
	C16-N10	1.363	N7-C15	1.309
	N10-C13	1.352	C11-H12	1.078
	C13-N6	1.311	N9-H4	1.007
	N6-N5	1.361	C13-H14	1.078
ωB97XD/def2-TZVP	N5-C16	1.309	N10-H1	1.007
	C15-N9	1.363	C16-N2	1.391
	N9-C11	1.352	C15-N3	1.391
	C11-N8	1.311	N2-N3	1.246
	N8-N7	1.361		
E1	Bond	Length (Å)	Bond	Length (Å)
	N6-N16	1.324	N9-N2	1.325
	N16-C7	1.316	C13-H14	1.077
	C7-C13	1.408	C7-H8	1.077
	C13-N10	1.317	C11-H12	1.077
ωB97XD/6-31G(d)	N10-N6	1.325	C1-H3	1.077
	N2-N15	1.324	N4-N2	1.364
	N15-C1	1.316	N5-N6	1.364
	C1-C11	1.408	N4-N5	1.227
	C11-N9	1.317		
E1	Bond	Length (Å)	Bond	Length (Å)
	N6-N16	1.331	N9-N2	1.333
	N16-C7	1.321	C13-H14	1.080
	C7-C13	1.412	C7-H8	1.079
	C13-N10	1.322	C11-H12	1.080
ωB97XD/6-31G(d,p)	N10-N6	1.333	C1-H3	1.079
	N2-N15	1.331	N4-N2	1.369
	N15-C1	1.321	N5-N6	1.369
	C1-C11	1.412	N4-N5	1.238
	C11-N9	1.322		
E1	Bond	Length (Å)	Bond	Length (Å)
	N6-N16	1.331	N9-N2	1.333
	N16-C7	1.321	C13-H14	1.079
ωB97XD/6-311G(d,p)	C7-C13	1.412	C7-H8	1.079
	C13-N10	1.322	C11-H12	1.079
	N10-N6	1.333	C1-H3	1.079

	N2-N15	1.331	N4-N2	1.369
	N15-C1	1.321	N5-N6	1.369
	C1-C11	1.412	N4-N5	1.238
	C11-N9	1.322		
E1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/def2-TZVP	N6-N16	1.328	N9-N2	1.330
	N16-C7	1.318	C13-H14	1.078
	C7-C13	1.411	C7-H8	1.078
	C13-N10	1.319	C11-H12	1.078
	N10-N6	1.330	C1-H3	1.078
	N2-N15	1.328	N4-N2	1.367
	N15-C1	1.318	N5-N6	1.367
	C1-C11	1.411	N4-N5	1.231
	C11-N9	1.319		
F1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-31G(d)	N4-C13	1.353	N5-N1	1.347
	C13-N16	1.303	C9-H10	1.078
	N16-C9	1.365	C13-H14	1.078
	C9-N6	1.309	C7-H8	1.078
	N6-N4	1.347	C11-H12	1.078
	N1-C11	1.353	N4-N3	1.359
	C11-N15	1.303	N1-N2	1.359
	N15-C7	1.365	N2-N3	1.228
	C7-N5	1.309		
F1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-31G(d,p)	N4-C13	1.359	N5-N1	1.354
	C13-N16	1.308	C9-H10	1.081
	N16-C9	1.369	C13-H14	1.080
	C9-N6	1.315	C7-H8	1.081
	N6-N4	1.354	C11-H12	1.080
	N1-C11	1.359	N4-N3	1.364
	C11-N15	1.308	N1-N2	1.364
	N15-C7	1.369	N2-N3	1.239
	C7-N5	1.315		
F1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/6-311G(d,p)	N4-C13	1.359	N5-N1	1.353
	C13-N16	1.308	C9-H10	1.080
	N16-C9	1.369	C13-H14	1.080
	C9-N6	1.315	C7-H8	1.080
	N6-N4	1.353	C11-H12	1.080
	N1-C11	1.359	N4-N3	1.364
	C11-N15	1.308	N1-N2	1.364
	N15-C7	1.369	N2-N3	1.239

	C7-N5	1.315		
F1	Bond	Length (Å)	Bond	Length (Å)
ωB97XD/def2-TZVP	N4-C13	1.358	N5-N1	1.350
	C13-N16	1.304	C9-H10	1.079
	N16-C9	1.368	C13-H14	1.079
	C9-N6	1.311	C7-H8	1.079
	N6-N4	1.350	C11-H12	1.079
	N1-C11	1.358	N4-N3	1.362
	C11-N15	1.304	N1-N2	1.362
	N15-C7	1.368	N2-N3	1.232
	C7-N5	1.311		

Table S2. The various enthalpies of azobis-triazole derivatives.

No.	ΔH_1[a] (kJ/mol)	ΔH_2[b] (kJ/mol)	ΔH_f[c] (solid) (kJ/mol)	ΔH_f[c] (solid) (kJ/g)	No.	ΔH_1[a] (kJ/mol)	ΔH_2[b] (kJ/mol)	ΔH_f[c] (solid) (kJ/mol)	ΔH_f[c] (solid) (kJ/g)
A1	56.60	1045.07	988.47	6.02	**B1**	58.95	956.98	898.03	5.47
A2	37.41	1394.00	1356.59	2.94	**B2**	49.36	1340.64	1291.28	2.79
A3	45.83	1118.03	1072.2	4.03	**B3**	61.39	1071.25	1009.86	3.79
A4	50.61	1240.75	1190.14	4.19	**B4**	58.73	1166.37	1107.64	3.90
A5	54.57	1153.07	1098.5	4.32	**B5**	54.06	1122.11	1068.05	4.20
A6	46.54	1042.42	995.88	3.48	**B6**	64.03	960.36	896.33	3.13
A1-NO(1)	59.99	1066.01	1006.01	5.58	**B1-NO(1)**	64.52	966.07	901.55	5.01
A2-NO(1)	39.76	1418.33	1378.57	2.88	**B2-NO(1)**	45.27	1355.49	1310.22	2.74
A3-NO(1)	49.21	1140.86	1091.65	3.87	**B3-NO(1)**	62.91	1083.84	1020.93	3.62
A4-NO(1)	52.29	1262.79	1210.5	4.03	**B4-NO(1)**	60.36	1177.14	1116.78	3.72
A5-NO(1)	56.71	1176.04	1119.33	4.14	**B5-NO(1)**	53.42	1134.02	1080.6	4.00
A6-NO(1)	49.26	1064.19	1014.93	3.36	**B6-NO(1)**	63.68	974.29	910.61	3.01
A1-NO(2)	65.01	1057.39	992.38	5.06	**B1-NO(2)**	66.64	980.81	914.16	4.66
A2-NO(2)	49.48	1424.56	1375.08	2.78	**B2-NO(2)**	55.37	1393.44	1338.08	2.71
A3-NO(2)	63.98	1165.24	1101.26	3.69	**B3-NO(2)**	69.75	1119.98	1050.23	3.52

A4-NO(2)	54.12	1262.21	1208.09	3.82	**B4-NO(2)**	65.55	1208.68	1143.13	3.62
A5-NO(2)	59.55	1221.00	1161.44	4.06	**B5-NO(2)**	119.21	1172.95	1053.73	3.68
A6-NO(2)	62.29	1066.89	1004.60	3.16	**B6-NO(2)**	72.79	991.95	919.15	2.89
C1	67.26	894.50	827.24	5.04	**D1**	78.12	804.07	725.95	4.42
C2	42.65	1233.01	1190.36	2.58	**D2**	49.28	1169.96	1120.68	2.42
C3	58.63	978.21	919.58	3.46	**D3**	66.64	896.31	829.67	3.12
C4	53.86	1089.82	1035.96	3.65	**D4**	67.39	991.17	923.78	3.25
C5	57.61	1028.56	970.95	3.82	**D5**	57.69	920.11	862.42	3.39
C6	56.79	883.27	826.48	2.89	**D6**	70.08	799.50	729.42	2.55
C1-NO(1)	69.54	841.58	772.03	4.29	**D1-NO(1)**	80.78	763.59	682.81	3.79
C2-NO(1)	44.42	1198.82	1154.4	2.41	**D2-NO(2)**	53.53	1132.36	1078.83	2.26
C3-NO(1)	58.63	949.45	890.82	3.16	**D3-NO(2)**	69.73	858.16	788.43	2.79
C4-NO(1)	53.85	1048.48	994.63	3.31	**D4-NO(2)**	64.96	952.65	887.69	2.96
C5-NO(1)	60.51	986.37	925.86	3.43	**D5-NO(2)**	61.17	883.03	821.86	3.04
C6-NO(1)	56.88	850.64	793.76	2.63	**D6-NO(2)**	72.80	760.16	687.36	2.28
C1-NO(2)	78.01	932.66	854.65	4.36	**D1-NO(2)**	85.73	836.47	750.74	3.83
C2-NO(2)	57.89	1307.70	1249.81	2.53	**D2-NO(2)**	58.73	1196.78	1138.05	2.30
C3-NO(2)	75.81	1048.46	972.65	3.26	**D3-NO(2)**	77.09	942.92	865.83	2.90

C4-NO(2)	66.58	1133.10	1066.52	3.37	**D4-NO(2)**	70.62	1029.08	958.46	3.03
C5-NO(2)	69.25	1109.94	1040.69	3.64	**D5-NO(2)**	63.86	971.30	907.45	3.17
C6-NO(2)	78.97	943.49	864.52	2.72	**D6-NO(2)**	79.89	817.39	737.49	2.32
E1	58.39	1010.36	951.97	5.80	**F1**	52.72	889.84	837.12	5.10
E2	36.49	1371.24	1334.75	2.89	**F2**	36.23	1279.03	1242.79	2.69
E3	43.51	1088.13	1044.61	3.93	**F3**	45.25	1005.10	959.85	3.61
E4	52.13	1212.64	1160.51	4.08	**F4**	53.48	1107.72	1054.24	3.71
E5	48.98	1123.56	1074.58	4.23	**F5**	47.86	1064.51	1016.65	4.00
E6	45.87	1011.32	965.45	3.37	**F6**	44.30	891.89	847.59	2.96
E1-NO(1)	56.43	1039.50	983.07	5.46	**F1-NO(1)**	54.56	919.32	864.76	4.80
E2-NO(1)	36.49	1371.24	1334.75	2.79	**F2-NO(2)**	38.13	1310.86	1272.73	2.66
E3-NO(1)	42.45	1122.69	1080.25	3.83	**F3-NO(2)**	46.64	1038.99	992.34	3.52
E4-NO(1)	51.85	1245.03	1193.18	3.98	**F4-NO(2)**	55.10	1137.29	1082.20	3.61
E5-NO(1)	51.53	1153.82	1102.29	4.08	**F5-NO(2)**	48.96	1082.05	1033.09	3.82
E6-NO(1)	46.02	1042.14	996.12	3.30	**F6-NO(2)**	46.07	926.23	880.17	2.91
E1-NO(2)	62.54	1103.04	1040.50	5.31	**F1-NO(2)**	64.07	1006.91	942.84	4.81
E2-NO(2)	41.84	1465.68	1423.83	2.88	**F2-NO(2)**	50.64	1411.02	1360.38	2.75
E3-NO(2)	54.33	1203.01	1148.68	3.85	**F3-NO(2)**	62.70	1140.91	1078.21	3.62

E4-NO(2)	53.15	1321.14	1267.99	4.01	**F4-NO(2)**	59.04	1222.11	1163.07	3.68
E5-NO(2)	51.57	1246.61	1195.04	4.18	**F5-NO(2)**	58.39	1207.05	1148.65	4.01
E6-NO(2)	56.39	1112.36	1055.97	3.32	**F6-NO(2)**	62.38	1009.27	946.89	2.98

[a] ΔH_1, the enthalpy of sublimation; [b] ΔH_2, the enthalpy of gas-phase formation; [c] ΔH_f, the enthalpy of solid formation

Table S3. Calculation results of detonation velocity (V_D (m/s)), detonation pressure (P (GPa)), detonation heat (Q (kJ/kg)), oxygen balance (Ω (%)) of azobis-triazole and its derivatives with different azo linkages.

No.	Ω[a]	V_D[b]	P[c]	Q[d]	No.	Ω[a]	V_D[b]	P[c]	Q[d]
A1	-97.47	7937.6	22.14	5774	**B1**	-97.47	7848.9	21.53	5251
A2	-3.46	9445.8	39.62	7777	**B2**	-3.46	9662.8	42.32	7706
A3	-42.08	8385.0	29.95	7477	**B3**	-42.08	8679.9	33.03	7271
A4	-33.78	9008.3	34.15	6697	**B4**	-33.78	9094.1	35.11	6452
A5	-31.48	9147.3	36.16	6929	**B5**	-31.48	9145.6	36.43	6827
A6	-16.77	9345.0	38.77	7114	**B6**	-16.77	9577.3	41.47	6895
A1-NO(1)	-79.94	8303.51	26.23	6414	**B1-NO(1)**	-79.94	8293.20	25.90	5882
A2-NO(1)	0	9504.6	40.52	7805	**B2-NO(1)**	0	9684.1	42.64	7731
A3-NO(1)	-34.02	8882.3	36.34	7674	**B3-NO(1)**	-34.02	9160.6	40.10	7479
A4-NO(1)	-26.65	9281.9	37.64	7039	**B4-NO(1)**	-26.65	9412.2	39.11	6784
A5-NO(1)	-23.69	9488.5	40.50	7315	**B5-NO(1)**	-23.69	9432.4	39.84	7179
A6-NO(1)	-10.59	9512.6	39.94	7594	**B6-NO(1)**	-10.59	9824.4	43.60	7280
A1-NO(2)	-65.26	8669.16	30.37	6801	**B1-NO(2)**	-65.26	8602.37	29.67	6432
A2-NO(2)	3.24	9702.61	42.91	7715	**B2-NO(2)**	3.24	9859.34	44.91	7679
A3-NO(2)	-26.83	9403.51	44.80	7922	**B3-NO(2)**	-26.83	9494.2	46.39	7784
A4-NO(2)	-20.24	9503.8	40.49	7283	**B4-NO(2)**	-20.24	9668.87	42.36	7132
A5-NO(2)	-16.77	9816.86	44.59	7742	**B5-NO(2)**	-16.77	9753.88	43.72	7407
A6-NO(2)	-5.03	9818.91	44.37	7949	**B6-NO(2)**	-5.03	10032.55	47.09	7741
C1	-97.47	7965.2	22.36	4841	**D1**	-97.47	8177.4	23.73	4240
C2	-3.46	9594.0	41.63	7515	**D2**	-3.46	9545.4	41.03	7382
C3	-42.08	8604.0	32.23	6945	**D3**	-42.08	8676.5	32.92	6623
C4	-33.78	8982.6	33.81	6208	**D4**	-33.78	9293.9	36.94	5883
C5	-31.48	9121.2	35.98	6490	**D5**	-31.48	8966.0	34.34	6088
C6	-16.77	9446.3	40.06	6656	**D6**	-16.77	9542.8	41.03	6389
C1-NO(1)	-79.94	8242.89	25.31	5203	**D1-NO(1)**	-79.94	8515.91	27.11	4739
C2-NO(1)	0	9678.5	42.34	7473	**D2-NO(1)**	0	9651.6	42.36	7341

C3-NO(1)	-34.02	8976.0	38.08	7034	**D3-NO(1)**	-34.02	9077.6	39.60	6704
C4-NO(1)	-26.65	9219.1	36.86	6388	**D4-NO(1)**	-26.65	9141.1	36.04	6057
C5-NO(1)	-23.69	9447.8	39.74	6693	**D5-NO(1)**	-23.69	9302.8	38.08	6330
C6-NO(1)	-10.59	9657.8	41.61	6897	**D6-NO(1)**	-10.59	9831.9	44.72	6608
C1-NO(2)	-65.26	8871.13	31.61	6183	**D1-NO(2)**	-65.26	9047.687	33.06	5698
C2-NO(2)	3.24	9979.39	46.38	7548	**D2-NO(2)**	3.24	9830.34	44.39	7343
C3-NO(2)	-26.83	9583.566	47.99	7557	**D3-NO(2)**	-26.83	9508.381	46.61	7217
C4-NO(2)	-20.24	9704.322	42.53	6920	**D4-NO(2)**	-20.24	9681.209	42.26	6608
C5-NO(2)	-16.77	9970.53	46.33	7423	**D5-NO(2)**	-16.77	9692.069	42.94	6957
C6-NO(2)	-5.03	10275.33	50.32	7607	**D6-NO(2)**	-5.03	10172.55	48.73	7228
E1	-97.47	7879.2	21.80	5563	**F1**	-97.47	7559.4	19.62	4891
E2	-3.46	9431.6	39.63	7737	**F2**	-3.46	9447.0	39.73	7582
E3	-42.08	8349.4	29.62	7382	**F3**	-42.08	9594.3	40.78	8225
E4	-33.78	9012.6	34.30	6606	**F4**	-33.78	8947.0	33.60	6261
E5	-31.48	9036.9	35.09	6821	**F5**	-31.48	8984.6	34.70	6615
E6	-16.77	9314.1	38.52	7019	**F6**	-16.77	9202.9	37.37	6649
E1-NO(1)	-79.94	8186.5	25.25	6284	**F1-NO(1)**	-79.94	7985.0	23.65	5664
E2-NO(1)	0	9467.3	39.92	7776	**F2-NO(1)**	0	9554.3	41.02	7645
E3-NO(1)	-34.02	8777.3	35.01	7623	**F3-NO(1)**	-34.02	9810.8	46.12	8474
E4-NO(1)	-26.65	9259.5	37.43	6984	**F4-NO(1)**	-26.65	9273.4	37.48	6658
E5-NO(1)	-23.69	9381.7	39.13	7231	**F5-NO(1)**	-23.69	9339.3	38.68	7005
E6-NO(1)	-10.59	9448.5	39.18	7531	**F6-NO(1)**	-10.59	9429.9	39.13	7164
E1-NO(2)	-65.26	8698.9	30.61	7024	**F1-NO(2)**	-65.26	8590.4	29.40	6561
E2-NO(2)	3.24	9594.2	41.62	7773	**F2-NO(2)**	3.24	9761.9	43.70	7700
E3-NO(2)	-26.83	9277.9	42.61	8038	**F3-NO(2)**	-26.83	10173.2	54.05	8926
E4-NO(2)	-20.24	9519.9	40.94	7454	**F4-NO(2)**	-20.24	9544.5	40.97	7166
E5-NO(2)	-16.77	9721.9	43.36	7810	**F5-NO(2)**	-16.77	9816.9	44.40	7703
E6-NO(2)	-5.03	9714.4	42.83	8068	**F6-NO(2)**	-5.03	9778.3	43.64	7788

[a] Ω, oxygen balance; [b] V_D, detonation velocity; [c] P, detonation pressure; [d] Q, detonation heat.

Table S4. Calculation results of the bond dissociation enthalpy (BDE(C-R) without *N*-Oxides, R = $C(NO_2)_3$, NF_2, $NHNO_2$, NO_2, ONO_2) and Mayer bond order (MBO) of azobis-triazole derivatives.

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$ (Hartree)	E_{AB} (Hartree)	BDE(C-R) (kJ/mol)	MBO
A2	-1244.4683	-653.2228	-1897.8707	471.35	0.913
A3	-845.4578	-254.2729	-1099.8503	313.88	0.813
A4	-851.5620	-260.3186	-1112.0594	469.32	0.909
A5	-796.2390	-205.0583	-1001.4120	301.08	0.754
A6	-871.4203	-280.1911	-1151.7759	431.82	0.980
B2	-1244.4966	-653.2228	-1897.8909	450.44	0.891
B3	-845.4847	-254.2729	-1099.8681	290.22	0.834
B4	-851.5941	-260.3186	-1112.0877	459.53	0.945
B5	-796.2622	-205.0583	-1001.4238	270.98	0.730
B6	-871.4539	-280.1911	-1151.8071	425.66	0.768
C2	-1244.5295	-653.2228	-1897.9319	471.73	0.905
C3	-845.5137	-254.2729	-1099.9035	307.10	0.826
C4	-851.6199	-260.3186	-1112.1169	468.44	0.923
C5	-796.2919	-205.0583	-1001.4594`	286.50	0.747
C6	-871.4801	-280.1911	-1151.8365	434.03	0.875
D2	-1244.5583	-653.2228	-1897.9559	459.03	0.903
D3	-845.5475	-254.2729	-1099.9347	300.30	0.838
D4	-851.6571	-260.3186	-1112.1545	469.40	0.912
D5	-796.3307	-205.0583	-1001.5007	293.18	0.739
D6	-871.5139	-280.1911	-1151.8684	429.12	0.872
E2	-1244.4808	-653.2228	-1897.8793	461.20	0.890
E3	-845.4721	-254.2729	-1099.8617	306.35	0.843
E4	-851.5750	-260.3186	-1112.0701	463.34	0.898
E5	-796.2523	-205.0583	-1001.4232	295.48	0.734
E6	-871.4340	-280.1911	-1151.7877	427.10	0.817
F2	-1244.5214	-653.2228	-1897.9144	446.98	0.871
F3	-845.5099	-254.2729	-1099.8933	290.05	0.817
F4	-851.6179	-260.3186	-1112.1101	455.54	0.938
F5	-796.2864	-205.0583	-1001.4457	265.15	0.709
F6	-871.4795	-280.1911	-1151.8332	426.99	1.023

Table S5. Calculation results of the bond dissociation enthalpy (BDE(N=N) without *N*-Oxides) and Mayer bond order (MBO) of azobis-triazole derivatives.

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE (N=N) (kJ/mol)	MBO
A1	-296.1420	-296.1420	-592.4428	416.64	1.750
A2	-948.8547	-948.8547	-1897.8706	423.01	1.665
A3	-549.8449	-549.8449	-1099.8503	421.49	1.666
A4	-555.9502	-555.9502	-1112.0594	417.40	1.659
A5	-500.6258	-500.6258	-1001.4120	420.98	1.667
A6	-575.8078	-575.8078	-1151.7759	420.49	1.665
B1	-296.1580	-296.1580	-592.47632	420.73	1.741
B2	-948.8632	-948.8632	-1897.8909	432.15	1.729
B3	-549.8539	-549.8539	-1099.8681	420.91	1.650
B4	-555.9624	-555.9624	-1112.0877	427.81	1.681
B5	-500.6341	-500.6341	-1001.4238	408.48	1.669
B6	-575.8229	-575.8229	-1151.8071	423.34	1.667
C1	-296.1724	-296.1724	-592.5001	407.53	1.617
C2	-948.8814	-948.8814	-1897.9319	444.20	1.591
C3	-549.8739	-549.8739	-1099.9035	408.72	1.554
C4	-555.9785	-555.9785	-1112.1169	419.68	1.571
C5	-500.6530	-500.6530	-1001.4594	402.48	1.612
C6	-575.8386	-575.8386	-1151.8365	418.38	1.557
D1	-296.1869	-296.1869	-592.5346	421.84	1.657
D2	-948.8960	-948.8960	-1897.9559	430.12	1.645
D3	-549.8858	-549.8858	-1099.9347	428.36	1.639
D4	-555.9984	-555.9984	-1112.1545	413.90	1.625
D5	-500.6687	-500.6687	-1001.5007	428.75	1.641
D6	-575.8537	-575.8537	-1151.8684	422.43	1.635
E1	-296.1479	-296.1479	-592.4560	420.45	1.626
E2	-948.8583	-948.8583	-1897.8793	426.83	1.639
E3	-549.8507	-549.8507	-1099.8617	420.84	1.636
E4	-555.9553	-555.9553	-1112.0701	418.70	1.620
E5	-500.6307	-500.6307	-1001.4232	424.76	1.636
E6	-575.8132	-575.8132	-1151.7877	423.63	1.631
F1	-296.1688	-296.1688	-592.5019	431.61	1.654
F2	-948.8730	-948.8730	-1897.9144	441.90	1.729
F3	-549.8659	-549.8659	-1099.8933	423.83	1.659
F4	-555.9728	-555.9728	-1112.1101	431.80	1.692
F5	-500.6456	-500.6456	-1001.4457	405.86	1.681
F6	-575.8344	-575.8344	-1151.8332	431.59	1.688

Table S6. Calculation results of the bond dissociation enthalpy (BDE(C-R)$_1$, BDE(C-R)$_2$, and BDE(N=N)$_1$with *N*-Oxide, which is located on the azo bond) and Mayer bond order (MBO) of azobis-triazole derivatives.

BDE(C-R)$_1$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_1$ (kJ/mol)	MBO
A1-*N*O(1)	–	–	–	–	–
A2-*N*O(1)	-1319.619754	-653.2227753	-1973.022199	471.72	0.915
A3-*N*O(1)	-920.609939	-254.2728934	-1175.002466	314.10	0.815
A4-*N*O(1)	-926.7144272	-260.3186097	-1187.21187	469.53	0.914
A5-*N*O(1)	-871.3905922	-205.058329	-1076.564087	302.38	0.754
A6-*N*O(1)	-946.5729657	-280.1910576	-1226.928438	431.67	0.989

BDE(C-R)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
A1-*N*O(1)	–	–	–	–	–
A2-*N*O(1)	-1319.62194	-653.2227753	-1973.022199	465.98	0.909
A3-*N*O(1)	-920.6109437	-254.2728934	-1175.002466	311.46	0.812
A4-*N*O(1)	-926.7150701	-260.3186097	-1187.21187	467.84	0.906
A5-*N*O(1)	-871.392468	-205.058329	-1076.564087	297.44	0.75
A6-*N*O(1)	-946.5733575	-280.1910576	-1226.928438	430.64	0.978

BDE(N=N)$_1$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_1$ (kJ/mol)	MBO
A1-*N*O(1)	-296.1420419	-371.3260113	-667.5956648	335.04	1.418
A2-*N*O(1)	-1024.040159	-948.8547374	-1973.022199	334.23	1.408
A3-*N*O(1)	-625.0293899	-549.8448938	-1175.002466	336.54	1.414
A4-*N*O(1)	-631.134636	-555.9501988	-1187.21187	333.53	1.411
A5-*N*O(1)	-575.8111251	-500.62581	-1076.564087	333.84	1.412
A6-*N*O(1)	-650.9922921	-575.8078519	-1226.928438	336.83	1.415

BDE(C-R)$_1$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_1$ (kJ/mol)	MBO
B1-*N*O(1)	–	–	–	–	–
B2-*N*O(1)	-1319.650873	-653.2227753	-1973.046132	452.86	0.894
B3-*N*O(1)	-920.6385705	-254.2728934	-1175.024186	295.95	0.829
B4-*N*O(1)	-926.7490543	-260.3186097	-1187.244494	464.27	0.943
B5-*N*O(1)	-871.4171387	-205.058329	-1076.580093	274.69	0.741
B6-*N*O(1)	-946.6088011	-280.1910576	-1226.962676	427.48	0.797

BDE(C-R)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
B1-*N*O(1)	–	–	–	–	–
B2-*N*O(1)	-1319.654036	-653.2227753	-1973.046132	444.55	0.889
B3-*N*O(1)	-920.6429325	-254.2728934	-1175.024186	284.50	0.823
B4-*N*O(1)	-926.751076	-260.3186097	-1187.244494	458.96	0.935
B5-*N*O(1)	-871.4194362	-205.058329	-1076.580093	268.66	0.736
B6-*N*O(1)	-946.6109727	-280.1910576	-1226.962676	421.78	0.75

BDE(N=N)$_1$					
No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_1$ (kJ/mol)	MBO
B1-*N*O(1)	-296.1580425	-371.3413456	-667.6337269	352.71	1.42
B2-*N*O(1)	-1024.04598	-948.8631611	-1973.046132	359.67	1.457
B3-*N*O(1)	-625.0375264	-549.8547236	-1175.024186	346.40	1.413
B4-*N*O(1)	-631.1465814	-555.9623908	-1187.244494	355.81	1.423
B5-*N*O(1)	-575.8154462	-500.634089	-1076.580093	342.78	1.411
B6-*N*O(1)	-651.0062252	-575.8229375	-1226.962676	350.54	1.432
BDE(C-R)$_1$					
No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_1$ (kJ/mol)	MBO
C1-*N*O(1)	–	–	–	–	–
C2-*N*O(1)	-1319.703445	-653.2227753	-1973.105804	471.50	0.902
C3-*N*O(1)	-920.6895226	-254.2728934	-1175.07537	296.56	0.819
C4-*N*O(1)	-926.7982754	-260.3186097	-1187.293495	463.69	0.924
C5-*N*O(1)	-871.4670855	-205.058329	-1076.63633	291.21	0.767
C6-*N*O(1)	-946.6562342	-280.1910576	-1227.009768	426.58	0.979
BDE(C-R)$_2$					
No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
C1-*N*O(1)	–	–	–	–	–
C2-*N*O(1)	-1319.703536	-653.2227753	-1973.105804	471.26	0.899
C3-*N*O(1)	-920.6865222	-254.2728934	-1175.07537	304.44	0.83
C4-*N*O(1)	-926.7967563	-260.3186097	-1187.293495	467.68	0.932
C5-*N*O(1)	-871.4699326	-205.058329	-1076.63633	283.73	0.745
C6-*N*O(1)	-946.6537415	-280.1910576	-1227.009768	433.13	0.988
BDE(N=N)$_1$					
No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_1$ (kJ/mol)	MBO
C1-*N*O(1)	-296.1724438	-371.373997	-667.6811462	353.67	1.445
C2-*N*O(1)	-1024.086346	-948.8813621	-1973.105804	362.57	1.436
C3-*N*O(1)	-625.0762362	-549.8723549	-1175.07537	332.86	1.422
C4-*N*O(1)	-631.1800979	-555.9785173	-1187.293495	354.13	1.44
C5-*N*O(1)	-575.8581409	-500.653045	-1076.63633	328.57	1.43
C6-*N*O(1)	-651.0402254	-575.8385514	-1227.009768	343.92	1.418
BDE(C-R)$_1$					
No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_1$ (kJ/mol)	MBO
D1-*N*O(1)	–	–	–	–	–
D2-*N*O(1)	-1319.733271	-653.2227753	-1973.131117	459.65	0.906
D3-*N*O(1)	-920.7231932	-254.2728934	-1175.11014	299.45	0.836
D4-*N*O(1)	-926.832817	-260.3186097	-1187.329998	468.84	0.915
D5-*N*O(1)	-871.505618	-205.058329	-1076.675687	293.37	0.74
D6-*N*O(1)	-946.6904166	-280.1910576	-1227.044233	427.32	1.029
BDE(C-R)$_2$					
No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
D1-*N*O(1)	–	–	–	–	–

D2-*N*O(1)	-1319.735239	-653.2227753	-1973.131117	454.48	0.895
D3-*N*O(1)	-920.7239447	-254.2728934	-1175.11014	297.47	0.832
D4-*N*O(1)	-926.8336035	-260.3186097	-1187.329998	466.77	0.91
D5-*N*O(1)	-871.5073507	-205.058329	-1076.675687	288.82	0.732
D6-*N*O(1)	-946.6903379	-280.1910576	-1227.044233	427.53	1.045

BDE(N=N)$_1$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_1$ (kJ/mol)	MBO
D1-*N*O(1)	-296.1869425	-371.3927118	-667.7108498	344.45	1.434
D2-*N*O(1)	-1024.104087	-948.8960503	-1973.131117	343.89	1.43
D3-*N*O(1)	-625.092654	-549.8857932	-1175.11014	345.76	1.432
D4-*N*O(1)	-631.2026354	-555.9984084	-1187.329998	338.57	1.425
D5-*N*O(1)	-575.8766772	-500.6686345	-1076.675687	342.30	1.425
D6-*N*O(1)	-651.0596279	-575.8537433	-1227.044233	343.58	1.428

BDE(C-R)$_1$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_1$ (kJ/mol)	MBO
E1-*N*O(1)	–	–	–	–	–
E2-*N*O(1)	-1319.628199	-653.2227753	-1973.028101	465.05	0.895
E3-*N*O(1)	-920.6185646	-254.2728934	-1175.009386	309.62	0.792
E4-*N*O(1)	-926.723672	-260.3186097	-1187.218634	463.01	0.904
E5-*N*O(1)	-871.4000409	-205.058329	-1076.572551	299.78	0.739
E6-*N*O(1)	-946.5824426	-280.1910576	-1226.93683	428.82	0.981

BDE(C-R)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
E1-*N*O(1)	–	–	–	–	–
E2-*N*O(1)	-1319.631554	-653.2227753	-1973.028101	456.24	0.886
E3-*N*O(1)	-920.6208321	-254.2728934	-1175.009386	303.67	0.788
E4-*N*O(1)	-926.7244159	-260.3186097	-1187.218634	461.06	0.899
E5-*N*O(1)	-871.4029737	-205.058329	-1076.572551	292.08	0.731
E6-*N*O(1)	-946.5838389	-280.1910576	-1226.93683	425.16	0.969

BDE(N=N)$_1$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_1$ (kJ/mol)	MBO
E1-*N*O(1)	-296.1479234	-371.3332499	-667.6057596	327.10	1.382
E2-*N*O(1)	-948.8583439	-1024.045515	-1973.028101	326.20	1.372
E3-*N*O(1)	-549.8506959	-625.0357166	-1175.009386	322.87	1.376
E4-*N*O(1)	-555.9553116	-631.1395195	-1187.218634	325.04	1.374
E5-*N*O(1)	-500.6307105	-575.8174712	-1076.572551	326.53	1.374
E6-*N*O(1)	-575.8131728	-650.9987618	-1226.93683	327.91	1.377

BDE(C-R)$_1$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_1$ (kJ/mol)	MBO
F1-*N*O(1)	–	–	–	–	–
F2-*N*O(1)	-1319.668145	-653.2227753	-1973.063131	452.14	0.878
F3-*N*O(1)	-920.6558871	-254.2728934	-1175.041269	295.34	0.834
F4-*N*O(1)	-926.7655215	-260.3186097	-1187.25967	460.88	0.939

F5-*N*O(1)	-871.4437201	-205.058329	-1076.599888	256.88	0.719
F6-*N*O(1)	-946.6268843	-280.1910576	-1226.980979	428.05	1.036

BDE(C-R)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
F1-*N*O(1)	–	–	–	–	–
F2-*N*O(1)	-1319.67334	-653.2227753	-1973.063131	438.50	0.865
F3-*N*O(1)	-920.6615721	-254.2728934	-1175.041269	280.41	0.83
F4-*N*O(1)	-926.7702673	-260.3186097	-1187.25967	448.42	0.923
F5-*N*O(1)	-871.4427862	-205.058329	-1076.599888	259.33	0.723
F6-*N*O(1)	-946.6300412	-280.1910576	-1226.980979	419.77	1.064

BDE(N=N)$_1$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_1$ (kJ/mol)	MBO
F1-*N*O(1)	-296.1687509	-371.3539854	-667.6515353	338.16	1.42
F2-*N*O(1)	-948.8730369	-1024.057161	-1973.063131	349.02	1.425
F3-*N*O(1)	-549.865938	-625.0510725	-1175.041269	326.24	1.396
F4-*N*O(1)	-555.9727989	-631.1582185	-1187.25967	337.78	1.396
F5-*N*O(1)	-500.6455555	-575.8267488	-1076.599888	334.97	1.403
F6-*N*O(1)	-575.8344006	-651.0193497	-1226.980979	334.04	1.434

Table S7. Calculation results of the bond dissociation enthalpy (BDE(C-R)$_2$ and BDE(N=N)$_2$) and Mayer bond order (MBO) of azobis-triazole derivatives with *N*-Oxide groups in azoles.

BDE(C-R)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
A1-*N*O(2)	–	–	–	–	–
A2-*N*O(2)	-1394.74254	-653.2227753	-2048.180697	565.49	0.885
A3-*N*O(2)	-995.7299387	-254.2728934	-1250.154052	397.03	0.820
A4-*N*O(2)	-1001.840543	-260.3186097	-1262.372962	561.35	0.914
A5-*N*O(2)	-946.5276208	-205.058329	-1151.707837	320.01	0.765
A6-*N*O(2)	-1021.71963	-280.1910576	-1302.088276	466.26	0.751

BDE(N=N)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_2$ (kJ/mol)	MBO
A1-*N*O(2)	-371.2985604	-371.2985604	-742.7598199	427.17	1.579
A2-*N*O(2)	-1024.008117	-1024.008117	-2048.180697	431.80	1.589
A3-*N*O(2)	-624.9943891	-624.9943891	-1250.154052	433.93	1.583
A4-*N*O(2)	-631.1060815	-631.1060815	-1262.372962	422.18	1.576
A5-*N*O(2)	-575.7717336	-575.7717336	-1151.707837	431.55	1.583
A6-*N*O(2)	-650.9624788	-650.9624788	-1302.088276	428.79	1.580

BDE(C-R)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
B1-*N*O(2)	–	–	–	–	–
B2-*N*O(2)	-1394.82997	-653.2227753	-2048.192549	367.05	0.912
B3-*N*O(2)	-995.8192748	-254.2728934	-1250.171293	207.74	0.884
B4-*N*O(2)	-1001.929818	-260.3186097	-1262.393354	380.50	1.005
B5-*N*O(2)	-946.5961685	-205.058329	-1151.726137	188.09	0.821
B6-*N*O(2)	-1021.791591	-280.1910576	-1302.116821	352.27	0.896

BDE(N=N)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_2$ (kJ/mol)	MBO
B1-*N*O(2)	-371.3124138	-371.3124138	-742.7889879	431.00	1.583
B2-*N*O(2)	-1024.015188	-1024.015188	-2048.192549	425.78	1.698
B3-*N*O(2)	-625.0072756	-625.0072756	-1250.171293	411.52	1.623
B4-*N*O(2)	-631.117077	-631.117077	-1262.393354	417.98	1.655
B5-*N*O(2)	-575.7862862	-575.7862862	-1151.726137	403.18	1.645
B6-*N*O(2)	-650.9789683	-650.9789683	-1302.116821	417.15	1.635

BDE(C-R)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
C1-*N*O(2)	–	–	–	–	–
C2-*N*O(2)	-1394.825086	-653.2227753	-2048.225209	465.63	0.865
C3-*N*O(2)	-995.8093328	-254.2728934	-1250.198531	305.36	0.832
C4-*N*O(2)	-1001.915561	-260.3186097	-1262.422139	493.51	0.947
C5-*N*O(2)	-946.585756	-205.058329	-1151.750136	278.44	0.745
C6-*N*O(2)	-1021.75342	-280.1910576	-1302.135279	500.95	1.095

BDE(N=N)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_2$ (kJ/mol)	MBO
C1-*N*O(2)	-371.3228477	-371.3228477	-742.8073251	424.36	1.593
C2-*N*O(2)	-1024.032206	-1024.032206	-2048.225209	422.17	1.568
C3-*N*O(2)	-625.018855	-625.018855	-1250.198531	422.24	1.569
C4-*N*O(2)	-631.128344	-631.128344	-1262.422139	434.39	1.575
C5-*N*O(2)	-575.7979648	-575.7979648	-1151.750136	404.87	1.569
C6-*N*O(2)	-650.9881736	-650.9881736	-1302.135279	417.28	1.559

BDE(C-R)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
D1-*N*O(2)	–	–	–	–	–
D2-*N*O(2)	-1394.894119	-653.2227753	-2048.267456	395.30	0.922
D3-*N*O(2)	-995.8796536	-254.2728934	-1250.23873	226.27	0.891
D4-*N*O(2)	-1001.992453	-260.3186097	-1262.461759	395.65	0.938
D5-*N*O(2)	-946.6615709	-205.058329	-1151.802939	218.02	0.8
D6-*N*O(2)	-1021.852435	-280.1910576	-1302.183308	367.08	1.239

BDE(N=N)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_2$ (kJ/mol)	MBO
D1-*N*O(2)	-371.3437213	-371.3437213	-742.8439647	410.95	1.579
D2-*N*O(2)	-1024.051886	-1024.051886	-2048.267456	429.75	1.611
D3-*N*O(2)	-625.0383873	-625.0383873	-1250.23873	425.21	1.599
D4-*N*O(2)	-631.1543347	-631.1543347	-1262.461759	401.94	1.567
D5-*N*O(2)	-575.8191266	-575.8191266	-1151.802939	432.38	1.61
D6-*N*O(2)	-651.0751842	-651.0751842	-1302.308617	415.48	1.572

BDE(C-R)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
E1-*N*O(2)	–	–	–	–	–
E2-*N*O(2)	-1394.75454	-653.2227753	-2048.165036	492.86	0.88
E3-*N*O(2)	-995.7415343	-254.2728934	-1250.139666	328.81	0.814
E4-*N*O(2)	-1001.847018	-260.3186097	-1262.350517	485.43	0.911
E5-*N*O(2)	-946.5208221	-205.058329	-1151.698082	312.25	0.769
E6-*N*O(2)	-1021.707187	-280.1910576	-1302.070958	453.46	1.066

BDE(N=N)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_2$ (kJ/mol)	MBO
E1-*N*O(2)	-371.2921202	-371.2921202	-742.7424307	415.33	1.604
E2-*N*O(2)	-1024.00243	-1024.00243	-2048.165036	420.54	1.614
E3-*N*O(2)	-624.989847	-624.989847	-1250.139666	420.01	1.611
E4-*N*O(2)	-631.0958828	-631.0958828	-1262.350517	416.80	1.609
E5-*N*O(2)	-575.7692267	-575.7692267	-1151.698082	419.10	1.61
E6-*N*O(2)	-650.9554906	-650.9554906	-1302.070958	420.02	1.611

BDE(C-R)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$(Hartree)	E_{AB} (Hartree)	BDE(C-R)$_2$ (kJ/mol)	MBO
F1-*N*O(2)	–	–	–	–	–
F2-*N*O(2)	-1394.821469	-653.2227753	-2048.185854	371.80	0.896

F3-*N*O(2)	-995.8094802	-254.2728934	-1250.163321	212.53	0.875
F4-*N*O(2)	-1001.921722	-260.3186097	-1262.388235	388.32	0.998
F5-*N*O(2)	-946.5843934	-205.058329	-1151.71315	184.91	0.775
F6-*N*O(2)	-1021.782644	-280.1910576	-1302.110223	358.44	1.199

BDE(N=N)$_2$

No.	$E_{A\cdot}$ (Hartree)	$E_{B\cdot}$·(Hartree)	E_{AB} (Hartree)	BDE(N=N)$_2$ (kJ/mol)	MBO
F1-*N*O(2)	-371.3096241	-371.3096241	-742.7790443	419.54	1.634
F2-*N*O(2)	-1024.010646	-1024.010646	-2048.185854	432.06	1.697
F3-*N*O(2)	-625.0032828	-625.0032828	-1250.163321	411.56	1.636
F4-*N*O(2)	-631.1136693	-631.1136693	-1262.388235	422.43	1.675
F5-*N*O(2)	-575.7813225	-575.7813225	-1151.71315	395.15	1.653
F6-*N*O(2)	-650.9756389	-650.9756389	-1302.110223	417.31	1.645

Figure S1. The effects of *N*-oxide groups on the density of different linkage modes of azobis-triazole derivatives.

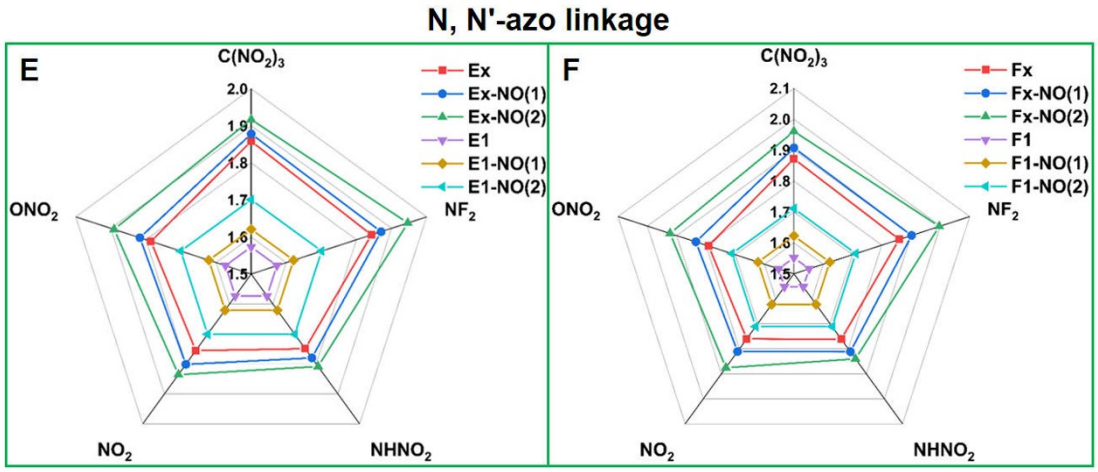

Figure S2a. The effects of *N*-oxide groups on the detonation pressure of different linkage modes of azobis-triazole derivatives.

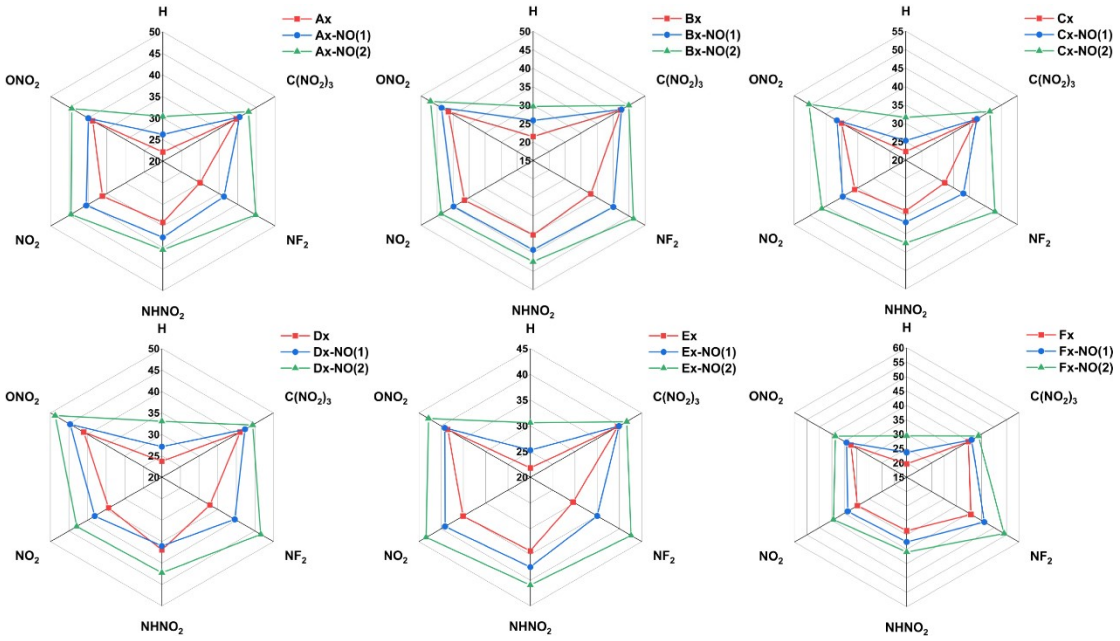

Figure S2b. The effects of *N*-oxide groups on the detonation heat of different linkage modes of azobis-triazole derivatives.

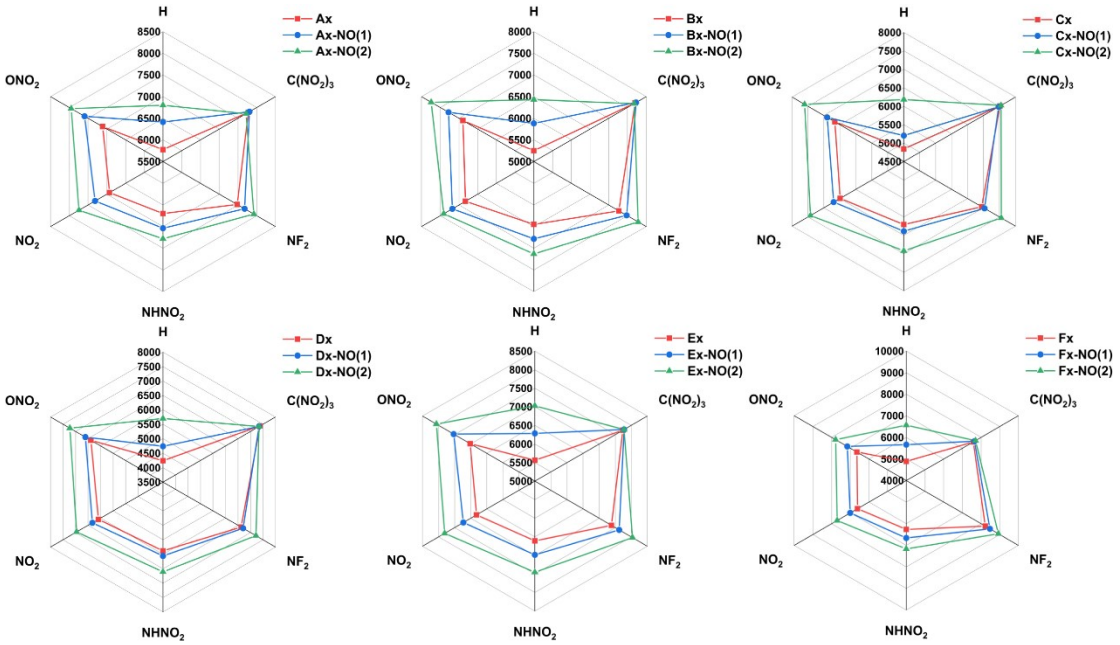

Figure S3. The effects of *N*-oxide groups on the azo bond dissociation enthalpy of different linkage modes of azobis-triazole derivatives.