Electronic Supplementary Information

Computational insight into the reactivity of FOX-7 and its bridge-ring energetic derivatives from Diels-Alder reactions

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Theoretical calculation methods

The electronic chemical potential (μ), global electrophilicity index(ω), and global nucleophilicity index (N) of FOX-7 and selected dienes were calculated by eqn (1)-(3). [1-2]

$$\mu = (E_{\mathrm{LUMO}} + E_{\mathrm{HOMO}}) / 2 \tag{1}$$

$$\omega = \mu^2 / 2(E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}}) \tag{2}$$

$$N = E_{\mathrm{HOMO}} - E_{\mathrm{LUMO\text{-}TCE}} \tag{3}$$

In which, HOMO and LUMO are the highest occupied molecular orbital and lowest unoccupied molecular orbital, respectively; and the HOMO and LUMO are analyzed at the B3LYP/6-31G(d) level. E_{HOMO} and E_{LUMO} are the energies of the HOMO and LUMO, respectively. TCE is tetracyanoethylene.

The solid-phase enthalpy of formation ($\Delta H_{\mathrm{f,\ solid}}$) was calculated according to Hess's law of constant heat summation(eqn (4)).[3] In which, gas-phase enthalpy of formation ($\Delta H_{\mathrm{f,\ gas}}$) was predicted via isodesmic reactions. The $\Delta H_{\mathrm{f,\ gas}}$ at 298K can be expressed as eqn (5) and aslo can be calculated by eqn (6) based on the isodesmic reaction. [4-6] The heat of sublimation (ΔH_{sub}) was calculated by the empirical formula eqn (7) proposed by Politzer et al. [7-8]

$$\Delta H_{\mathrm{f,\ solid}} = \Delta H_{\mathrm{f,\ gas}} - \Delta H_{\mathrm{sub}} \tag{4}$$

$$\Delta H_{\mathrm{f,\ gas}} = \sum \Delta H_{\mathrm{f,P}} - \sum \Delta H_{\mathrm{f,R}} \tag{5}$$

$$\Delta H_{\mathrm{f,\ gas}} = \Delta E + \Delta(PV) = \Delta E_0 + \Delta ZPE + \Delta H_{\mathrm{T}} + \Delta nRT \tag{6}$$

In which, $\Delta H_{\mathrm{f,P}}$ and $\Delta H_{\mathrm{f,R}}$ are the enthalpy of formation(HOF) of the products and reactants in the isodesmic reaction at 298 K, respectively; ΔE_0 is the change in total energy between the products and reactants at 0 K; ΔZPE is the difference between the the zero-point energy (ZPE) of the products and reactants at 0 K; ΔH_{T} is the thermal correction from 0 to 298 K; the Δ(PV) value is the PV work term and equals ΔnRT for the reactions of ideal gas, and Δn=0 for the isodesmic reactions. For the reference compounds without experimental HOF values, their HOF values were obtained by atomization reaction $C_aH_bO_cN_d(g) \rightarrow aC(g)+bH(g)+cO(g)+dN(g)$ using the highly accurate G2 method.

$$\Delta H_{\mathrm{sub}} = aA^2 + b(\nu\sigma_{\mathrm{tot}}^2)^{0.5} + c \tag{7}$$

In which, A represents the surface area of the 0.001 electrons per bohr^3 isosurface of electron density of the molecule; ν quantifies the degree of balance between the positive and negative potentials on the molecular surface; σ_{tot}^2 is the total variance of the electrostatic potential; the coefficients a, b and c were expressed as 2.670×10^{-4} kcal·mol^{-1}·Å^{-4}, 1.650 kcal·mol^{-1} and 2.966 kcal·mol^{-1}.[9] A, ν, and σ_{tot}^2 were calculated by the Multiwfn program. [10]

The crystal density (ρ) of the designed energetic compounds was calculated using the improved calculation formula (eqn (8)) proposed by Politzer et al. [11]

$$\rho = \alpha\left(\frac{M}{V_{\mathrm{m}}}\right) + \beta\left(\nu\sigma_{\mathrm{tot}}^2\right) + \gamma \tag{8}$$

In which, M is the molecular mass, g·mol^{-1}; V_{m} is the volume inside the 0.001 electrons per bohr^3 isosurface of electron density surrounding the molecule, cm^3·mol^{-1}; σ_{tot}^2 is the total variance of the electrostatic potential; ν quantifies the degree of balance between the positive and negative potentials on the molecular surface; the product

$v\sigma_{tot}^2$ proved to be an excellent index of electrostatic interactive tendencies; the fit parameters α, β and γ are 1.0462, 0.0021 and -0.1586, respectively [12].

Detonation velocity (D), detonation pressure (P), heat of detonation (Q) and strength (ΔV_{Trauzl}) are important parameters to characterize detonation performance of energetic materials. And the values of Q, D and P in this work were calculated by EXPLO5 (V6.05.04) program. The ΔV_{Trauzl} were estimated by eqn (9) for $C_aH_bO_cN_d$ compounds proposed by Keshavarz et al. [13]

$$\Delta V_{Trauzl} = 1101 - 19248(a / M_W) - 14925(d / M_W) + 64.13(\Delta H_{f,solid} / M_W) \quad (9)$$

In which, a and d are the number of C and N atoms in the molecule, respectively; M_W is the molecular weight; $\Delta H_{f,solid}$ is the solid-phase heat of formation, kJ·mol^{-1}.

Impact sensitivity is usually expressed as drop height marked h_{50} in cm. Here the h_{50} was predicted using eqn (10) proposed by Pospíšil et al. [14]

$$h_{50} = \alpha\sigma_+^2 + \beta\nu + \gamma \quad (10)$$

In which, σ_+^2 indicates the strengths and variabilities of the positive surface potentials; ν quantifies the degree of balance between the positive and negative potentials on the molecular surface; The coefficients α, β and γ are -0.0064, 241.42 and -3.43, respectively. [14-15]

Oxygen balance (OB) is an important parameter that describes the level of oxygen and closely related to the detonation performance for energetic compounds. The OB for $C_aH_bN_cO_d$ molecules with the molecular weight M_w can be calculated by eqn (11).

$$OB = 1600 \times (d - 2a - b/2) / M_W \quad (11)$$

Table S1 The E_{LUMO}, E_{HOMO}, μ, N and ω of the dienes

Compd.	E_{LUMO} (eV)	E_{HOMO} (eV)	μ (eV)	N (eV)	ω (eV)	Compd.	E_{LUMO} (eV)	E_{HOMO} (eV)	μ (eV)	N (eV)	ω (eV)
A0	-0.01	-6.85	-3.43	2.27	0.86						
AA1	0.72	-5.69	-2.49	3.43	0.48	**AN1**	-2.94	-7.94	-5.44	1.18	2.96
AA2	0.25	-5.6	-2.68	3.52	0.61	**AN2**	-2.56	-7.99	-5.28	1.13	2.57
AA3	0.5	-5.59	-2.55	3.53	0.53	**AN3**	-2.92	-8.07	-5.50	1.05	2.94
AA4	1.07	-4.97	-1.95	4.15	0.31	**AN4**	-3.63	-8.84	-6.24	0.28	3.73
AA5	0.75	-5.51	-2.38	3.61	0.45	**AN5**	-4.04	-8.94	-6.49	0.18	4.30
AA6	0.53	-5.4	-2.44	3.72	0.50	**AN6**	-3.75	-8.45	-6.10	0.67	3.96
AA7	1.13	-4.76	-1.82	4.36	0.28	**AN7**	-4.58	-9.04	-6.81	0.08	5.21
B0	-0.41	-7.3	-3.86	1.82	1.08						
BA1	0.04	-6.35	-3.16	2.77	0.78	**BN1**	-2.90	-8.34	-5.62	0.78	2.90
BA2	-0.17	-5.96	-3.07	3.16	0.81	**BN2**	-2.81	-8.44	-5.62	0.68	2.81
BA3	0.31	-5.95	-2.82	3.17	0.64	**BN3**	-3.19	-8.46	-5.83	0.66	3.22
BA4	0.3	-5.86	-2.78	3.26	0.63	**BN4**	-3.36	-8.84	-6.10	0.28	3.39
BA5	0.78	-5.69	-2.46	3.43	0.47	**BN5**	-3.90	-9.08	-6.49	0.04	4.07
BA6	0.37	-5.69	-2.66	3.43	0.58	**BN6**	-3.91	-8.78	-6.35	0.34	4.14
BA7	0.83	-5.54	-2.36	3.58	0.44	**BN7**	-4.40	-9.14	-6.77	-0.02	4.83
C0	-1.28	-7.82	-4.55	1.30	1.58						
CA1	-1.02	-6.31	-3.67	2.81	1.27	**CN1**	-3.02	-8.71	-5.87	0.41	3.03
CA2	-0.54	-6.38	-3.46	2.74	1.02	**CN2**	-3.70	-8.87	-6.29	0.25	3.82
D0	-0.99	-8.37	-4.68	0.75	1.48						
DA1	-0.44	-6.68	-3.56	2.44	1.02	**DN1**	-3.18	-8.64	-5.91	0.48	3.20
DA2	-0.04	-6.77	-3.41	2.35	0.86	**DN2**	-3.62	-8.91	-6.26	0.21	3.70
DA3	0.55	-6.06	-2.76	3.06	0.57	**DN3**	-4.29	-9.21	-6.75	-0.09	4.62
E0	-1.47	-8.8	-5.14	0.32	1.80						
EA1	-1.01	-6.87	-3.94	2.25	1.32	**EN1**	-3.48	-8.94	-6.21	0.18	3.53
EA2	-0.55	-6.45	-3.50	2.67	1.04	**EN2**	-3.84	-9.25	-6.54	-0.13	3.95
F0	-0.55	-7.9	-4.23	1.22	1.21						
FA1	0.13	-6.56	-3.22	2.56	0.77	**FN1**	-3.43	-8.79	-6.11	0.33	3.48
FA2	0.80	-5.73	-2.47	3.39	0.47	**FN2**	-4.39	-9.44	-6.92	-0.32	4.74

HOMO and LUMO are the highest occupied molecular orbital and lowest unoccupied molecular orbital, respectively; E_{HOMO} and E_{LUMO} are the energies of the HOMO and LUMO, respectively; μ, N and ω are electronic chemical potential, global nucleophilicity index and global electrophilicity index, respectively.

Table S2 Energy barrier for electron transfer between dienes and **FOX-7**

Compd.	$\|\Delta E_1\|$ (eV)	$\|\Delta E_2\|$ (eV)	Compd.	$\|\Delta E_1\|$ (eV)	$\|\Delta E_2\|$ (eV)
A0	4.56	7.05			
AA1	3.40	7.78	**AN1**	5.65	4.12
AA2	3.31	7.31	**AN2**	5.70	4.50
AA3	3.30	7.56	**AN3**	5.78	4.14
AA4	2.68	8.13	**AN4**	6.55	3.43
AA5	3.22	7.81	**AN5**	6.65	3.02
AA6	3.11	7.59	**AN6**	6.16	3.31
AA7	2.47	8.19	**AN7**	6.75	2.48
B0	5.01	6.65			
BA1	4.06	7.10	**BN1**	6.05	4.16
BA2	3.67	6.89	**BN2**	6.15	4.25
BA3	3.66	7.37	**BN3**	6.17	3.87
BA4	3.57	7.36	**BN4**	6.55	3.70
BA5	3.40	7.84	**BN5**	6.79	3.16
BA6	3.40	7.43	**BN6**	6.49	3.15
BA7	3.25	7.89	**BN7**	6.85	2.66
C0	5.53	5.78			
CA1	4.02	6.04	**CN1**	6.42	4.04
CA2	4.09	6.52	**CN2**	6.58	3.36
D0	6.08	6.07			
DA1	4.39	6.62	**DN1**	6.35	3.88
DA2	4.48	7.02	**DN2**	6.62	3.44
DA3	3.77	7.61	**DN3**	6.92	2.77
E0	6.51	5.59			
EA1	4.58	6.05	**EN1**	6.65	3.58
EA2	4.16	6.51	**EN2**	6.96	3.22
F0	5.61	6.51			
FA1	4.27	7.19	**FN1**	6.50	3.63
FA2	3.44	7.86	**FN2**	7.15	2.67

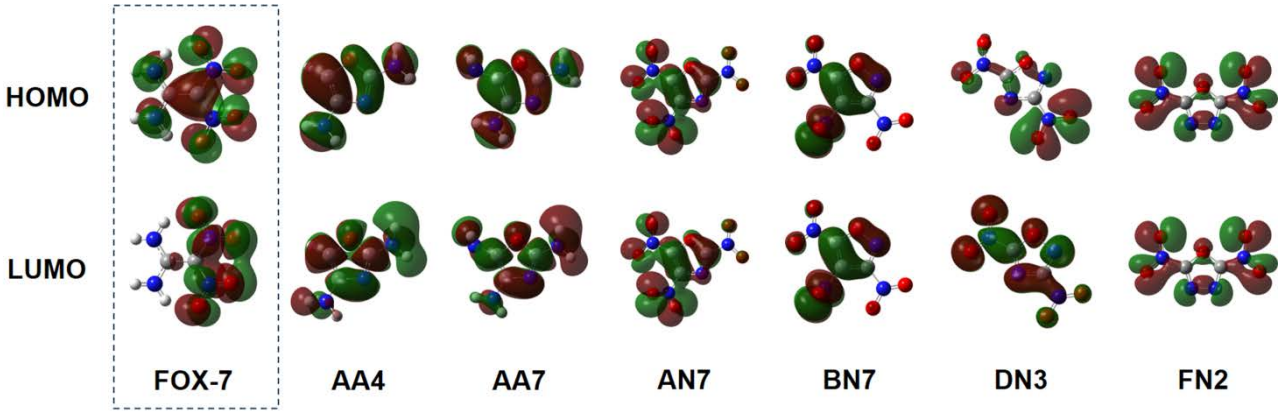


Fig. S1 The HOMO and LUMO pictures

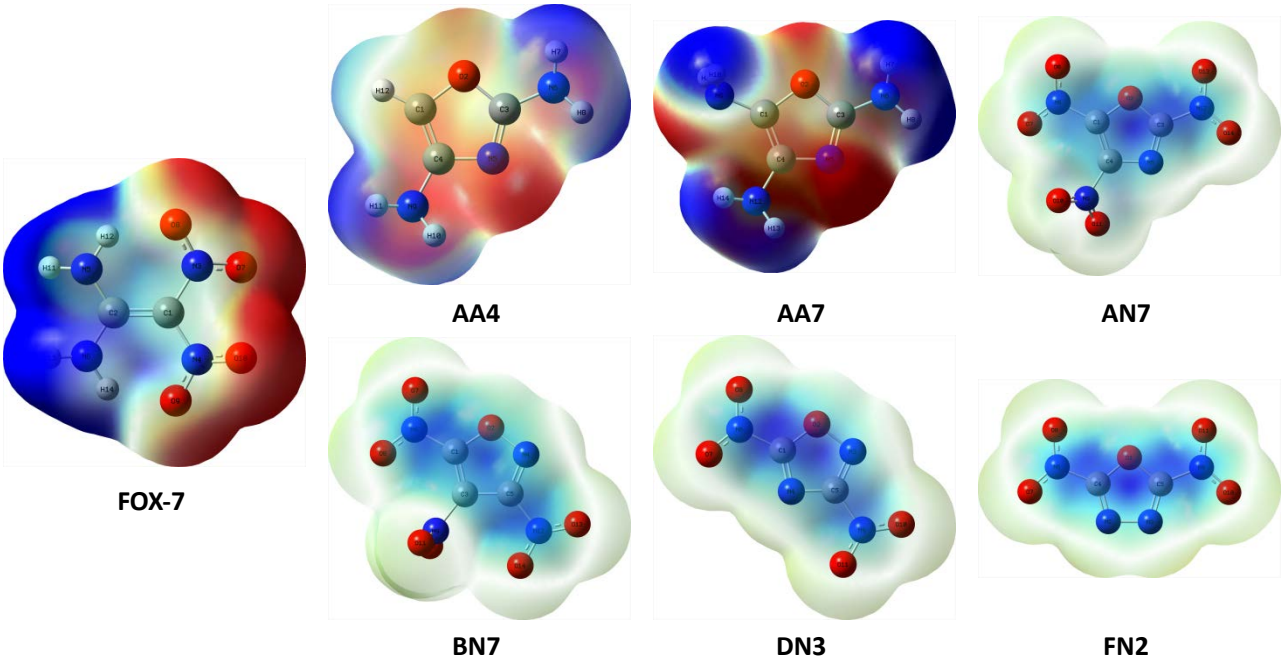


Fig. S2 The molecular surface electrostatic potential maps of preferred dienes and FOX-7

The Cartesian coordinates of transition states (TSs) and intermediate products (IMs):

(1) The Cartesian coordinates of TSs and IMs for the reaction between **FOX-7** and **AA4**

TS1 (for the formation of compound **P1-1**)

O	-0.05885900	-1.77121600	0.90794600
C	1.62065300	-1.19245900	-0.42665300
N	0.61588200	-1.61237500	-1.22841800
N	-1.59633500	-2.32266900	-0.68554800
H	-2.30204500	-2.08140900	0.00616900
H	-1.87249000	-2.13666300	-1.64163400
N	2.82838400	-0.82686500	-0.90469600
H	2.81308500	-0.50628500	-1.86621900
H	3.38605200	-0.25560000	-0.28215300
N	-1.76861100	0.50092300	0.24932100
N	-0.09597200	1.55696900	-1.11410600
N	0.10585700	0.81667300	2.49861600
N	1.80467900	1.48462800	1.10725400
O	-2.48413000	0.41949800	-0.74107800
O	-2.15089900	0.05220400	1.35075900
O	1.09489000	1.43331600	-1.45698000
O	-0.91005600	2.14673400	-1.79070000
H	0.81815100	0.54057300	3.16286200
H	-0.80160400	0.37843700	2.61867500
H	1.83232900	2.26472600	1.75780300
H	2.00934700	1.78568800	0.15970600
C	-0.46347400	1.00817600	0.14873100
C	1.17785000	-1.11686600	0.91244900
H	1.77028800	-1.25616200	1.80515300
C	-0.35699000	-1.90478400	-0.38291400
C	0.54898400	0.84617000	1.19223800

IM (for the formation of compound **P1-1**)

O	-0.05973500	1.75598200	0.82604200
C	-1.68673600	0.98369200	-0.51885300
N	-0.80693300	1.58534700	-1.30723000
N	1.38783600	2.34028300	-0.80511100
H	2.12674100	2.18014900	-0.11977600
H	1.63894200	2.28161000	-1.78366100
N	-2.86855400	0.52915800	-0.89108400
H	-3.03190300	0.41142900	-1.88424900
H	-3.31884100	-0.12718400	-0.26099700
N	1.82136700	-0.36898000	0.27416400
N	0.24231000	-1.59560200	-1.01298500
N	-0.08656400	-0.67824500	2.53992900

N	-1.75276500	-1.47222900	1.13807100
O	2.59308000	-0.38890500	-0.68409800
O	2.13027800	0.27080100	1.31167500
O	-0.94408400	-1.50324500	-1.41115700
O	1.07388400	-2.23797800	-1.62032700
H	-0.78289600	-0.29712200	3.17627900
H	0.79173300	-0.17258800	2.62433300
H	-1.59480800	-2.20286900	1.82927200
H	-1.83169000	-1.90902400	0.22250300
C	0.55088300	-0.92862300	0.19242900
C	-1.15799600	0.84648800	0.87731400
H	-1.85351400	1.13164400	1.66619600
C	0.19224400	1.90132200	-0.46672600
C	-0.57306700	-0.61078000	1.18296200

TS2 (for the formation of compound **P1-1**)

O	0.44345100	1.72391600	-0.79669900
C	2.03635500	0.63450000	0.35486500
N	1.25191000	1.13561800	1.25874300
N	-0.81598800	2.30209100	1.05043700
H	-1.64188300	2.45038600	0.47790300
H	-1.01163100	2.12636500	2.02766400
N	3.21563000	0.04595200	0.58806800
H	3.46481800	-0.16391700	1.54521300
H	3.68051200	-0.45848400	-0.15164000
N	-1.94614100	0.12993400	-0.23775400
N	-0.57497600	-1.40155700	1.01691500
N	-0.20620700	-0.70704300	-2.42292300
N	1.27069200	-1.77532200	-1.02393100
O	-2.73138500	0.10509100	0.69583000
O	-2.16751600	0.74961200	-1.27825800
O	0.46795200	-1.50508900	1.65561500
O	-1.50610500	-2.17087400	1.10585100
H	0.51460500	-0.78169000	-3.13659300
H	-0.80949000	0.08808800	-2.60438100
H	0.73453600	-2.58186700	-1.33925700
H	1.56911300	-1.94028500	-0.06575100
C	-0.60132200	-0.32764600	0.00968500
C	1.36357400	0.67011000	-0.99987200
H	1.98166200	0.82825800	-1.88267400
C	0.12057000	1.47810100	0.51640100
C	0.43118000	-0.60436800	-1.13709400

TS1 (for the formation of compound **P1-2**)

O	1.23524900	-0.31370800	-1.46897600
C	0.80024600	1.73348200	-0.70807300
N	1.73342200	1.25654700	0.08069100
N	2.96527700	-0.85176400	0.05629000
H	3.79980400	-0.37945500	-0.28510900
H	3.03255800	-0.90062000	1.07487300
N	0.32482500	3.01254500	-0.68544100
H	0.38567500	3.44009800	0.23149700
H	-0.58004600	3.15045600	-1.11648100
N	-1.58684500	-0.96361600	-0.84678200
N	-1.50980300	0.57066300	1.01908600
N	0.58610600	-2.34169300	0.63165800
N	0.85098600	-0.58709900	2.09120000
O	-2.56242700	-0.35166700	-1.24496300
O	-1.19718200	-2.01439500	-1.34432300
O	-0.89302900	1.52267100	1.49182000
O	-2.66119200	0.30735100	1.28474000
H	1.55182900	-2.59978800	0.81160000
H	0.27979200	-2.68413700	-0.27053500
H	0.34610200	-1.13634100	2.78318600
H	0.74720000	0.40793600	2.26609600
C	-0.75212000	-0.32897600	0.15374600
C	0.34585100	0.66406600	-1.54945300
H	-0.35234900	0.65357900	-2.37822600
C	1.82290700	-0.08405200	-0.22142200
C	0.42816800	-0.95499000	0.77683600

TS1 (for the formation of compound **P1-3**)

O	-1.21273500	-0.28128000	-1.49841900
C	-0.74020000	1.72574000	-0.67892900
N	-1.72533400	1.27158000	0.06717100
N	-3.04550900	-0.72657300	-0.09073800
H	-2.88439100	-1.69266400	0.19199400
H	-3.68880000	-0.22063500	0.50324300
N	-0.19711500	2.97221200	-0.56946100
H	-0.34962000	3.40475700	0.33425700
H	0.75435700	3.07090100	-0.90106000
N	1.38164600	0.83499000	0.74444100
N	1.67000300	-1.19234900	-0.51662000
N	-0.74283800	-0.77132300	2.14299400
N	-0.75837600	-2.30505900	0.42205800
O	2.30082600	1.32321600	0.10705300
O	0.90150400	1.35108100	1.74540500

O	1.25274600	-1.78861800	-1.50251900
O	2.78096900	-1.31743300	-0.04994000
H	-1.71220300	-1.03366200	2.30584600
H	-0.57054300	0.17975800	2.44730100
H	-0.34474000	-2.95092200	1.09174600
H	-0.46847400	-2.53463700	-0.52457100
C	0.71927000	-0.32020700	0.17912500
C	-0.25473100	0.64505800	-1.49303500
H	0.48887800	0.61794100	-2.27836300
C	-1.86376800	-0.04266800	-0.28459800
C	-0.44195200	-0.96140800	0.78044500

TS1 (for the formation of compound **P1-4**)

O	-0.29115800	-1.01598300	1.64831200
C	-1.94107600	-0.76706600	0.17978900
N	-1.14703200	-1.74757500	-0.29506000
N	0.93593400	-2.57140700	0.50748800
H	1.73999100	-2.22577700	1.02279100
H	1.12334800	-2.95079500	-0.41212600
N	-3.08636600	-0.41434300	-0.44139600
H	-3.09630800	-0.60738300	-1.43653500
H	-3.49656400	0.47071400	-0.17941200
N	0.23631000	0.36830500	-1.65215900
N	1.99577200	0.36500700	-0.01579400
N	-1.09697600	2.36537100	0.09614300
N	0.25712600	1.81281500	1.85333400
O	0.88140500	-0.40459000	-2.33624700
O	-0.88215300	0.78911000	-2.01124100
O	2.23754700	0.08779400	1.17705500
O	2.85676600	0.31306600	-0.87228100
H	-1.72941500	2.74014200	0.79093500
H	-1.46129000	2.18528600	-0.83065100
H	0.59324300	2.77128800	1.79641800
H	1.00246200	1.19652800	2.16690400
C	0.67538500	0.75216200	-0.36665100
C	-1.34086600	-0.15043400	1.30699400
H	-1.83245100	0.31614000	2.14849700
C	-0.15807300	-1.80073000	0.58320800
C	-0.22297900	1.41631200	0.58341300

IM (for the formation of compound **P1-4**)

O	-0.04965800	1.76923900	-0.81132400
C	-1.67368100	0.99022700	0.53064100
N	-0.78531000	1.57017000	1.32028100

N	1.41750400	2.30353500	0.82321100
H	2.15242600	2.12435900	0.13555800
H	1.66556700	2.22768900	1.80155100
N	-2.87627800	0.59753400	0.92375200
H	-3.01780200	0.49118100	1.92194900
H	-3.38718500	-0.04036000	0.32857500
N	0.14323500	-1.63776000	0.96609400
N	1.81758500	-0.39595500	-0.18465800
N	-1.54106000	-1.59012400	-1.32888600
N	-0.05248500	-0.39180100	-2.59202600
O	0.91666600	-2.32028900	1.60366100
O	-1.06400300	-1.52494500	1.28664900
O	2.19083900	0.29581400	-1.17055700
O	2.54397400	-0.48799600	0.80424100
H	-2.19061300	-1.37377200	-2.07724400
H	-1.97653600	-1.83549500	-0.44929900
H	0.20349900	-1.32168900	-2.92380200
H	0.80921900	0.15084100	-2.55962500
C	0.53901600	-0.93327200	-0.19383300
C	-1.15265500	0.85809900	-0.87184000
H	-1.83354800	1.15579900	-1.66910000
C	0.21633300	1.88711800	0.48037200
C	-0.52733200	-0.57256000	-1.22939000

TS2 (for the formation of compound **P1-4**)

O	-0.52113600	-0.14939700	1.90086100
C	-2.07073500	-0.39893800	0.29134600
N	-1.40366900	-1.51993400	0.30960600
N	0.59189900	-2.13155000	1.45848000
H	1.45741000	-1.74711100	1.82765600
H	0.70289600	-2.88801200	0.79359300
N	-3.19973500	-0.18905300	-0.38854300
H	-3.45581600	-0.86409900	-1.09740700
H	-3.58559900	0.73928400	-0.46052300
N	0.37591800	-0.53924600	-1.55874200
N	2.02845700	0.21789100	-0.00351800
N	-0.75881400	2.13788100	-0.97739100
N	0.42657700	2.29432600	0.98338200
O	1.11820700	-1.46009700	-1.86102500
O	-0.66779800	-0.28419700	-2.16711100
O	2.30723300	0.18127500	1.20041600
O	2.85690200	0.33180200	-0.88012400
H	-1.31206300	2.90895900	-0.61739300
H	-1.23645900	1.58769400	-1.68012900

H	1.11227600	2.80899100	0.43261500
H	0.91803200	1.80428500	1.72758400
C	0.61593000	0.14759000	-0.33154200
C	-1.32551400	0.66206100	1.05729900
H	-1.88726600	1.40077000	1.62702800
C	-0.29181500	-1.19810800	1.06512400
C	-0.24205000	1.35438700	0.10776000

(2) The Cartesian coordinates of TSs and IMs for the reaction between **FOX-7** and **AA7**

TS1 (for the formation of compound **P2-1**)

C	-1.40851400	0.19016700	0.78582000
O	-0.35126200	0.82719900	1.51380700
C	0.05435100	1.81480900	0.72477600
C	-1.64953600	1.11047500	-0.27471900
N	-0.70700800	2.07074400	-0.32757300
N	1.17513100	2.47243900	1.05788800
H	1.55980200	3.02824300	0.30406600
H	1.86306600	1.91660700	1.56017300
N	-2.42187900	-0.43148400	1.50979500
H	-2.04709500	-1.14999000	2.12297500
H	-2.97546600	0.21802200	2.06449600
N	-2.65093300	1.01203500	-1.15992900
H	-2.51529000	1.49812600	-2.03755900
H	-3.09788400	0.10313100	-1.20348000
N	1.74773100	-0.72498400	0.70214900
N	1.21993500	-0.18830300	-1.59185300
N	-0.62303000	-2.46472600	0.68835600
N	-1.34986900	-1.61146100	-1.28647800
O	2.67436600	0.08263000	0.67834300
O	1.51596900	-1.40106600	1.71864100
O	0.29512800	0.13081400	-2.36519100
O	2.38611600	0.02435000	-1.86185000
H	-0.00085000	-2.45275400	1.48723500
H	-1.58779300	-2.73390800	0.83608000
H	-1.43052400	-2.60219600	-1.49208800
H	-1.05472500	-1.08133400	-2.10084700
C	0.87124000	-0.85517400	-0.38998300
C	-0.46859400	-1.42614200	-0.20548300

IM (for the formation of compound **P2-1**)

C	-1.28800300	0.10296000	-0.68769200
O	-0.29124900	-0.54439400	-1.55205500
C	0.00598100	-1.68333700	-0.95425600
C	-1.64062100	-1.08091900	0.18129700

N	-0.84620400	-2.12046500	-0.01390000
N	1.10770900	-2.31230500	-1.31792300
H	1.39175200	-3.08798100	-0.73291100
H	1.85158400	-1.73554000	-1.70956000
N	-2.39261000	0.61406700	-1.39006700
H	-2.10452200	1.36617300	-2.00889800
H	-2.87431600	-0.09968900	-1.92971500
N	-2.65410500	-1.02541500	1.01689200
H	-2.75239600	-1.75547000	1.71147900
H	-3.01775100	-0.09373000	1.20911100
N	1.85118200	0.70345500	-0.52692800
N	1.12006700	0.00314800	1.63361700
N	-0.49459000	2.51505000	-0.55885100
N	-1.38860300	1.53810300	1.30862900
O	2.77707100	-0.11614000	-0.47477900
O	1.70136200	1.41678400	-1.53450800
O	0.11184000	-0.45343500	2.23122600
O	2.24721900	-0.19037800	2.05125500
H	0.12153600	2.49330000	-1.36322300
H	-1.43704900	2.83687000	-0.75584700
H	-1.23826700	2.51580500	1.54696200
H	-1.08811800	0.97046500	2.09844100
C	0.88677600	0.77023700	0.48146200
C	-0.52118500	1.27119900	0.16331800

TS2 (for the formation of compound **P2-1**)

C	1.51086700	-0.53662600	0.40177600
O	0.71648300	-1.68800300	0.03975000
C	0.08482300	-1.19468900	-1.06070000
C	1.80679900	-0.00951800	-0.98830600
N	0.92644100	-0.40987900	-1.85214800
N	-0.82764200	-2.00889500	-1.64015900
H	-1.28016700	-1.61324800	-2.45457700
H	-1.45102400	-2.48881000	-0.99695100
N	2.62224600	-0.75283400	1.22710800
H	2.30241200	-0.80103900	2.19524200
H	3.12324700	-1.59724600	0.96800800
N	2.80312100	0.85585600	-1.17452800
H	2.97215800	1.25552800	-2.08614200
H	3.47489500	0.97174500	-0.42660500
N	-1.96509900	-0.53361500	0.40118200
N	-1.17014300	1.54043400	-0.46273000
N	0.22294200	-0.13461700	2.42673400
N	0.93843700	1.73034900	1.22057300

O	-2.94105700	-0.38597900	-0.32044300
O	-1.86483700	-1.47386100	1.19956800
O	-0.42258200	1.99752600	-1.31349600
O	-2.11042600	2.14149000	0.02010800
H	-0.49449600	-0.85536200	2.42885000
H	-0.03634600	0.61196600	3.06405700
H	0.22913100	2.34677500	1.61627300
H	1.19309300	2.11426600	0.31337800
C	-0.80082500	0.23531200	0.11223400
C	0.41405800	0.39193100	1.09372400

TS1 (for the formation of compound **P2-2**)

C	-0.08335300	-1.76340800	-0.41683400
O	-1.17118000	-1.23006400	-0.91530600
C	-1.75898800	-0.52818400	0.17123600
C	-0.12759600	-1.63057700	1.00565100
N	-1.19892600	-0.94009800	1.33340600
N	-3.12519000	-0.33381000	0.02140500
H	-3.50536800	-0.02141000	0.90955400
H	-3.26501000	0.39642000	-0.68169800
N	0.84836900	-2.31513000	-1.20269300
H	0.86240300	-1.95506800	-2.15651500
H	1.76820100	-2.35520900	-0.77027600
N	0.92911000	-1.99957900	1.82885400
H	0.92691700	-1.44994900	2.68312900
H	0.97235600	-2.99379200	2.03042500
N	1.23459800	0.47420900	-1.32568700
N	1.37533200	1.12591300	0.98279900
N	-1.52254600	1.63128900	-1.31860700
N	-1.41634700	1.93409500	0.96991500
O	2.38423600	0.05246900	-1.25803700
O	0.58298700	0.40031700	-2.39003100
O	0.86179400	0.91040000	2.08727900
O	2.50197500	1.55519000	0.84913200
H	-0.97580500	1.52399500	-2.16479400
H	-2.02134100	2.50649900	-1.21840500
H	-1.16747900	2.92196700	0.92055500
H	-1.04476100	1.55180000	1.83562900
C	0.55725100	0.90947000	-0.18103800
C	-0.87054600	1.23437000	-0.14529000

IM (for the formation of compound **P2-2**)

C	0.16281800	1.67445600	-0.57126100
O	1.14019700	1.07264400	-1.12803100

C	1.74502500	0.21946100	0.03709400
C	0.37112200	1.68014000	0.90161900
N	1.36726100	0.92879400	1.20122800
N	3.09334300	0.04296500	-0.16962300
H	3.65066200	0.29733300	0.63433400
H	3.28326600	-0.88977800	-0.52843800
N	-0.82865300	2.22643700	-1.24608600
H	-0.96217100	1.84783300	-2.18697000
H	-1.69111600	2.38450600	-0.73286800
N	-0.49317500	2.29136200	1.74885800
H	-0.36416900	2.06786200	2.72791400
H	-0.78720100	3.23797300	1.54961000
N	-1.37989900	-0.46361900	-1.19580200
N	-1.36684100	-0.99222700	1.12757700
N	1.36226500	-1.76967400	-1.32381200
N	1.33427800	-1.95271100	0.99648800
O	-2.53273800	-0.03755500	-1.06973600
O	-0.81641100	-0.42163900	-2.31854200
O	-0.80424800	-0.66962900	2.18242100
O	-2.47755300	-1.48452300	1.09776200
H	0.83352000	-1.42047100	-2.12056100
H	1.22228000	-2.77489200	-1.25858300
H	0.86068200	-2.85489400	0.96709400
H	1.06647500	-1.50860300	1.87203500
C	-0.62321600	-0.80828700	-0.08900000
C	0.87654400	-1.13919500	-0.11284500

TS2 (for the formation of compound **P2-2**)

C	0.29957700	1.28069200	-0.90863700
O	1.18336800	0.45987400	-1.40312100
C	1.77491600	-0.13249800	-0.14773800
C	0.81895400	1.74107600	0.40777200
N	1.73791600	0.93571300	0.80611800
N	3.02640500	-0.67402100	-0.39563300
H	3.71428100	-0.34693600	0.26962700
H	2.97051700	-1.68829900	-0.44998500
N	-0.57855600	1.91255300	-1.70369400
H	-0.84459300	1.37230100	-2.52775500
H	-1.37833500	2.31635500	-1.22507400
N	0.28171500	2.79723600	1.05990300
H	0.64014200	2.97112900	1.98959800
H	0.04092900	3.61819100	0.52176600
N	-1.57289500	-0.51192900	-1.00422900
N	-1.40911000	-0.31379900	1.36538700

N	0.83375800	-2.32457900	-0.71387300
N	0.96825400	-1.69356000	1.52899100
O	-2.65139500	0.07380000	-0.92373900
O	-1.14172300	-0.93798100	-2.08832400
O	-0.87667200	0.38207500	2.22060600
O	-2.42656400	-0.95344900	1.54310300
H	0.34518200	-2.14408500	-1.58727500
H	0.47145700	-3.18094800	-0.30340500
H	0.25571600	-2.34256700	1.86026400
H	1.00333100	-0.91114500	2.17812100
C	-0.69545100	-0.45894600	0.09395400
C	0.64747900	-1.22229600	0.20216600

TS1 (for the formation of compound **P2-3**)

C	-1.06133500	-0.89200700	0.72503600
C	-1.65321700	0.61308300	-0.47941500
C	0.28766200	0.93946900	-1.40490600
C	0.39820600	-0.84122500	0.60358100
C	0.06481200	1.90181300	-0.35875600
O	-0.83175500	0.29660900	-1.61000600
N	-1.13720900	1.71228100	0.13220400
N	0.98343500	2.82544000	0.09143800
H	1.89489700	2.40172800	0.27405700
H	0.64576400	3.25341500	0.94904500
N	-3.00763900	0.45994300	-0.70645200
H	-3.32619200	-0.48431000	-0.49052800
H	-3.56244100	1.19640900	-0.29213000
N	-1.62471800	-0.62434700	1.97708600
H	-2.61813900	-0.43422800	1.87981600
H	-1.14113700	0.11880100	2.46889300
N	-1.79855300	-1.93215600	0.10709400
H	-1.33695400	-2.29132600	-0.72317800
H	-1.98097000	-2.66992800	0.78279600
N	1.10177100	-1.70837700	-0.28395100
O	0.51326300	-2.09316800	-1.30946900
O	2.23843600	-2.04760000	-0.02105400
N	1.20569800	0.08545800	1.29225400
O	0.72435900	0.68279500	2.26121600
O	2.33011700	0.36765700	0.85738200
N	1.38715700	0.65235200	-2.11447600
H	2.27139000	0.89251100	-1.67788600
H	1.37205400	-0.25438400	-2.57506300

IM (for the formation of compound **P2-3**)

C	-0.87654000	-1.13919800	-0.11284000
C	-1.74502600	0.21945500	0.03709000
C	-0.16282200	1.67445100	-0.57126900
C	0.62321800	-0.80828200	-0.08899600
C	-0.37113000	1.68014400	0.90161000
O	-1.14019900	1.07263400	-1.12803800
N	-1.36726700	0.92879600	1.20122100
N	0.49316300	2.29137500	1.74884800
H	0.36415300	2.06788200	2.72790500
H	0.78718600	3.23798500	1.54959400
N	-3.09334300	0.04295300	-0.16962800
H	-3.65066400	0.29732300	0.63432600
H	-3.28326200	-0.88979200	-0.52843900
N	-1.33427100	-1.95271000	0.99649800
H	-1.06647200	-1.50859400	1.87204300
H	-0.86067000	-2.85489000	0.96711000
N	-1.36225600	-1.76968600	-1.32380400
H	-0.83351300	-1.42048500	-2.12055400
H	-1.22226700	-2.77490300	-1.25856800
N	1.37990300	-0.46362100	-1.19579900
O	0.81641700	-0.42164800	-2.31854000
O	2.53274100	-0.03755400	-1.06973300
N	1.36684300	-0.99221600	1.12758300
O	0.80425100	-0.66961000	2.18242500
O	2.47755300	-1.48451500	1.09777100
N	0.82864800	2.22643300	-1.24609500
H	1.69111000	2.38450700	-0.73287800
H	0.96216800	1.84782600	-2.18697800

TS2 (for the formation of compound **P2-3**)

C	-0.64743700	-1.22232800	0.20214600
C	-1.77491400	-0.13259700	-0.14768300
C	-0.29965600	1.28074300	-0.90858800
C	0.69548700	-0.45895000	0.09395600
C	-0.81903000	1.74102900	0.40785800
O	-1.18339300	0.45989500	-1.40309600
N	-1.73794200	0.93560200	0.80618500
N	-0.28185300	2.79720200	1.06002400
H	-0.64034300	2.97105200	1.98970400
H	-0.04119300	3.61820000	0.52189500
N	-3.02634100	-0.67421200	-0.39558500
H	-3.71443100	-0.34671800	0.26924800
H	-2.97051500	-1.68851700	-0.44944300

N	-0.96819300	-1.69368400	1.52893900
H	-1.00292600	-0.91136200	2.17820000
H	-0.25585600	-2.34300600	1.86002000
N	-0.83371200	-2.32455800	-0.71396900
H	-0.34598300	-2.14340300	-1.58771300
H	-0.47011100	-3.18068600	-0.30411800
N	1.57288100	-0.51182900	-1.00427200
O	1.14168900	-0.93781100	-2.08838600
O	2.65138200	0.07390200	-0.92378600
N	1.40917600	-0.31382600	1.36536600
O	0.87667300	0.38191400	2.22066200
O	2.42672800	-0.95334200	1.54299800
N	0.57845700	1.91267600	-1.70360100
H	1.37822300	2.31649500	-1.22497200
H	0.84449500	1.37250400	-2.52771500

TS1 (for the formation of compound **P2-4**)

C	-1.55396000	0.42008700	0.65005200
O	-0.57220700	0.56856100	1.68190200
C	-0.00478000	-0.62733300	1.75191500
C	-1.64485000	-0.98578900	0.49486800
N	-0.63947000	-1.61427800	1.13143300
N	1.14495400	-0.74619300	2.43442700
H	1.68177200	0.11143600	2.52198100
H	1.67547400	-1.58129200	2.21639000
N	-2.62146200	1.29706000	0.55297500
H	-3.24851000	1.28842600	1.35314600
H	-2.27626700	2.24005100	0.36530400
N	-2.56813600	-1.62595000	-0.24552000
H	-2.27234100	-2.50133400	-0.65997800
H	-3.17842000	-1.04310000	-0.80183800
N	0.91610600	-1.11998100	-1.18302500
N	2.01776800	0.74263900	-0.13907200
N	-1.13150500	0.86060000	-2.08611000
N	-0.35246100	2.39509100	-0.57982600
O	1.80319700	-1.85352500	-0.78829100
O	-0.03372000	-1.54520600	-1.86700700
O	1.86583400	1.64200900	0.71602800
O	3.11689500	0.29572200	-0.40389600
H	-1.13350500	-0.09470200	-2.42492400
H	-2.05059000	1.27731800	-1.97311100
H	-0.29350200	2.98514300	-1.40420300
H	0.37898200	2.60109400	0.09633300
C	0.86963700	0.24266100	-0.80248600

C	-0.34665600	1.03929800	-0.96034100

IM (for the formation of compound **P2-4**)

C	-1.40817000	0.62322000	0.15195800
O	-0.61725100	1.15404800	1.27703100
C	-0.16596700	0.07778500	1.88797000
C	-1.66305800	-0.75949100	0.69481300
N	-0.85384800	-1.06492700	1.69311900
N	0.89553400	0.19785200	2.66211300
H	1.50346500	0.98879300	2.45495500
H	1.31201700	-0.65670800	3.00902900
N	-2.56577100	1.34129600	-0.16958900
H	-3.18083700	1.49154100	0.62431900
H	-2.28829900	2.22388400	-0.60197900
N	-2.64174600	-1.51587600	0.23339200
H	-2.61970100	-2.50639600	0.44326700
H	-3.09662800	-1.21759800	-0.62016100
N	0.92941800	-1.47918700	-0.75335800
N	2.07144900	0.55914600	-0.25280000
N	-0.93609200	0.19210300	-2.31595900
N	-0.20021000	2.10945600	-1.28964500
O	1.89890900	-2.14254600	-0.42323000
O	-0.16323600	-2.03184300	-1.04870000
O	1.93074900	1.65730200	0.34903600
O	3.17314300	0.05912300	-0.39183600
H	-1.00790100	-0.81982300	-2.30747700
H	-1.84190200	0.63021900	-2.46086300
H	0.19616000	2.22543500	-2.21982700
H	0.45938700	2.47946300	-0.60699500
C	0.91436300	-0.08344900	-0.72622300
C	-0.36140400	0.67751500	-1.08578200

TS2 (for the formation of compound **P2-4**)

C	-1.51149500	0.59227300	0.37076800
O	-0.71047900	0.68856500	1.57895300
C	-0.06708100	-0.50222600	1.52033300
C	-1.77064400	-0.89537200	0.36170000
N	-0.87896700	-1.53505400	1.06410100
N	0.90525400	-0.74091300	2.42545100
H	1.54265300	0.03923500	2.55356000
H	1.35622000	-1.63939200	2.29092500
N	-2.62961400	1.42442900	0.27119600
H	-3.22531500	1.38093700	1.09100800
H	-2.35344300	2.37880500	0.05541000

N	-2.75679100	-1.40879800	-0.36921800
H	-2.70717400	-2.39106600	-0.60603200
H	-3.17333600	-0.77587300	-1.04289800
N	1.04054300	-1.27653500	-0.87047600
N	2.01522200	0.73870600	-0.07046200
N	-1.00004700	0.60989000	-2.06030200
N	-0.18606200	2.31809500	-0.65619200
O	1.99159400	-1.89413600	-0.41602800
O	0.22072700	-1.76200800	-1.65012800
O	2.02613900	1.49285300	0.90554000
O	2.95606300	0.60286300	-0.82596400
H	-0.51245000	-0.12222100	-2.56133300
H	-1.07167700	1.46506600	-2.59905900
H	0.51104400	2.59590700	-1.34653300
H	0.20265700	2.53245900	0.26180300
C	0.77589100	0.01795600	-0.31817200
C	-0.42805400	0.88775300	-0.76371500

(3) The Cartesian coordinates of TSs and IMs for the reaction between **FOX-7** and **AN7**

TS1 (for the formation of compound **P3-1**)

C	1.61972400	-0.51399400	-0.94732000
O	0.30085600	-0.78209500	-1.29620200
C	-0.37139300	0.34699700	-0.93616000
C	1.63228300	0.80227100	-0.54444200
N	0.45493900	1.39468800	-0.62829700
N	2.40125600	-1.53073700	-0.40007800
O	1.90582300	-2.65582700	-0.27687400
O	3.52334100	-1.21488900	-0.02471000
N	2.74398300	1.47578800	0.12771700
O	2.72225900	1.35978100	1.34038700
O	3.54403000	2.07366000	-0.54282900
N	-1.46725900	0.68962300	-1.93342600
O	-1.30005000	0.29876900	-3.05786900
O	-2.35868000	1.38322500	-1.49855800
N	-2.65069400	-0.69348700	0.28761200
N	-1.48564500	1.18859000	1.38559000
N	-0.65961800	-2.39093400	0.89841400
N	0.59197700	-0.80867100	1.98181800
O	-2.64047300	-1.38036100	-0.72869200
O	-3.57460800	-0.54818100	1.03942000
O	-0.50355800	1.54319500	2.02484400
O	-2.50231600	1.81363000	1.25714500
H	-1.31155100	-2.59460400	0.14530800
H	0.11629100	-3.04247700	0.98213500

H	1.26623200	-1.51843300	2.24943800
H	0.79154700	0.16924300	2.19065900
C	-1.32322100	-0.07655600	0.61683400
C	-0.44040700	-1.12788600	1.22917400

IM (for the formation of compound **P3-1**)

C	1.65689300	0.00915100	1.10078500
O	0.29807100	0.15877400	1.42745300
C	-0.40448000	-0.64326300	0.53091300
C	1.65453400	-0.90686300	0.05631400
N	0.48130500	-1.34021800	-0.32201500
N	2.40208500	1.18675600	0.97691200
O	1.86172800	2.26612800	1.25839900
O	3.54732500	1.08123900	0.54994400
N	2.80154100	-1.16468500	-0.82001300
O	2.73633400	-0.57463000	-1.88876900
O	3.67233000	-1.89858800	-0.43963600
N	-1.24715500	-1.63468500	1.38282500
O	-0.59305600	-2.28324900	2.15447400
O	-2.44131400	-1.68515800	1.18530600
N	-2.66445800	0.67636900	0.27474300
N	-1.70355900	-0.39144100	-1.67997500
N	-0.70901800	2.62259200	0.11282600
N	0.55641900	1.43214400	-1.38817800
O	-2.56522600	1.11371100	1.40794600
O	-3.66114300	0.54980400	-0.37900800
O	-1.61935400	0.30355000	-2.67268000
O	-2.07258900	-1.52895200	-1.60102100
H	-1.35465700	2.56652400	0.89698700
H	0.05184500	3.28946100	0.21886000
H	1.26956200	2.15682600	-1.40526900
H	0.76094700	0.58201400	-1.91416200
C	-1.34085500	0.28564500	-0.36469000
C	-0.47487000	1.53471500	-0.58591400

TS2 (for the formation of compound **P3-1**)

C	-1.25886100	0.51940500	-0.67959500
O	-0.11342000	0.66589000	-1.45668500
C	0.57883100	-0.41980800	-0.93782200
C	-1.41482700	-0.88326700	-0.51514600
N	-0.32005000	-1.52217600	-0.74046800
N	-2.20272200	1.54005500	-0.61264900
O	-1.90070800	2.63301600	-1.07594100
O	-3.20819000	1.28649600	0.05198000

N	-2.58692900	-1.55110500	0.05651900
O	-2.69146800	-1.42994100	1.26160300
O	-3.30804500	-2.15458100	-0.69491700
N	1.73124900	-0.81333600	-1.82259800
O	1.68566800	-0.46616200	-2.97112300
O	2.56223300	-1.49663000	-1.26523300
N	2.31026100	0.93988800	0.44029400
N	1.36983100	-1.11096600	1.42543800
N	0.16003300	2.32869000	0.82043800
N	-0.74337600	0.70028700	2.19959100
O	2.56276900	1.38419500	-0.66152100
O	2.86997500	1.17738500	1.47578100
O	0.39979900	-1.67030700	1.90162300
O	2.51833100	-1.43481500	1.54284100
H	0.49926600	2.55926000	-0.11134100
H	-0.54609200	2.98098800	1.14584700
H	-1.48205500	1.34615600	2.45827200
H	-0.98153100	-0.27818500	2.33498100
C	1.05581300	0.07950200	0.53320000
C	-0.04982800	1.01350800	1.08920200

TS1 (for the formation of compound **P3-2**)

C	-0.26569700	-0.45721800	0.73982000
O	0.95653500	-0.22335700	1.28871900
C	1.80977200	-0.95869800	0.48223400
C	-0.07883700	-1.63750800	-0.07025100
N	1.22772000	-1.80322300	-0.30597200
N	-1.35347000	-0.39763600	1.79884700
O	-1.15644200	-1.15936900	2.71054700
O	-2.27519600	0.36393100	1.64346000
N	-1.09455900	-2.52405800	-0.53323000
O	-2.18390600	-2.40564600	0.01125700
O	-0.80135800	-3.32675100	-1.39717700
N	3.11830200	-0.44356300	0.36141900
O	3.50139900	0.32039400	1.23813500
O	3.73599300	-0.71281700	-0.66578000
N	-1.03577500	2.21036300	0.37186500
N	-1.48884700	0.71944500	-1.46500400
N	1.71944900	2.05718700	-0.20125000
N	1.29527000	0.76464800	-2.04856700
O	-2.04972600	2.72712100	-0.01600400
O	-0.38854900	2.51550600	1.36454100
O	-2.42247300	0.04593100	-1.12168800
O	-1.28402200	1.16342200	-2.58413700

H	2.68850200	2.16392700	-0.48178000
H	1.46707300	2.30870800	0.75176700
H	2.28669000	0.60570800	-2.20767700
H	0.63311400	0.35592900	-2.69522600
C	-0.49010100	1.05687600	-0.39291000
C	0.88318500	1.33266200	-0.92369600

IM (for the formation of compound **P3-2**)

C	-0.08503800	0.27893900	-0.61829400
O	1.06415400	-0.38967300	-0.99932100
C	2.13182300	0.36182600	-0.50675200
C	0.46366400	1.51324800	-0.00611500
N	1.79933000	1.47133900	0.05206500
N	-0.97273900	0.53104400	-1.86819600
O	-0.37323300	0.95361300	-2.82079000
O	-2.16012000	0.33666000	-1.75007100
N	-0.33197500	2.61044000	0.35791300
O	-1.54190400	2.45198600	0.15350600
O	0.18505600	3.60205000	0.83163400
N	3.31234800	-0.36222700	-0.19968400
O	3.19040000	-1.59140200	-0.09564500
O	4.33532200	0.25801600	-0.00572100
N	-1.67607400	-1.82722900	-0.36364500
N	-1.86543200	0.03373800	1.27790300
N	0.62362900	-2.63094700	0.67335000
N	0.87153500	-0.82465800	2.06340100
O	-2.61148700	-2.33156500	0.19289300
O	-1.16467000	-2.18164800	-1.41259200
O	-3.01178900	0.10849100	0.96044800
O	-1.33373800	0.55981000	2.24587500
H	1.56508500	-2.93175200	0.91360400
H	0.30455200	-2.95216500	-0.23812100
H	1.73461300	-1.20258800	2.44071800
H	0.49709500	0.05184000	2.42297200
C	-0.91235000	-0.73280300	0.37101500
C	0.22696300	-1.45230000	1.11137100

TS2 (for the formation of compound **P3-2**)

C	-0.47825800	0.22709900	-0.71896900
O	0.70481600	0.37880700	-1.42958700
C	1.42003500	1.08061500	-0.46324800
C	-0.54726500	1.53509300	0.02308000
N	0.66269100	1.94049900	0.23833000
N	-1.61093800	-0.12136300	-1.65290700

O	-1.67875300	0.55407800	-2.64364400
O	-2.33611400	-1.02540900	-1.30041500
N	-1.73175800	2.23155400	0.45928500
O	-2.75536800	1.92067300	-0.12322300
O	-1.60423400	3.06270500	1.33138900
N	2.81137800	1.07507300	-0.51292400
O	3.34264700	0.45260100	-1.42565500
O	3.39622400	1.52973500	0.47570400
N	-0.27628900	-2.30199100	-0.34508300
N	-1.11124900	-0.97353700	1.52285200
N	2.26221400	-1.51204300	0.30792900
N	1.52049400	-0.23713000	2.08856600
O	-0.93850100	-3.14876600	0.18158700
O	0.31679300	-2.37100200	-1.40338600
O	-2.09796400	-0.28158500	1.42768000
O	-0.80086500	-1.69203900	2.44236300
H	3.20468300	-1.40640300	0.67036300
H	2.20005600	-1.72195300	-0.68538300
H	2.43091500	0.21461200	2.18628600
H	0.77623700	0.30363700	2.51431100
C	-0.14172500	-0.94314900	0.35202700
C	1.29935800	-0.75561000	0.85870800

TS1 (for the formation of compound **P3-3**)

C	0.01369000	-0.33889400	0.69354700
O	-1.10936000	0.36506700	1.00974400
C	-2.14389400	-0.32864400	0.41762300
C	-0.48950000	-1.53524200	0.07520900
N	-1.81986000	-1.44638800	-0.12281800
N	0.95313700	-0.45005200	1.90109100
O	0.38686400	-0.76708400	2.91570500
O	2.13215900	-0.26595000	1.72533500
N	0.30804000	-2.65357300	-0.26761000
O	1.49629100	-2.54214900	0.03073300
O	-0.21376100	-3.60838200	-0.80240400
N	-3.34963100	0.39785300	0.19057600
O	-3.26546500	1.62497300	0.26501000
O	-4.34119600	-0.23173400	-0.10407800
N	1.91216600	-0.05990800	-1.24566000
N	1.68719700	1.87072800	0.29436100
N	-0.69909200	0.78237500	-2.24891000
N	-0.69584300	2.53399300	-0.76744800
O	3.06215000	-0.12090900	-0.92239300
O	1.38262600	-0.72781600	-2.13547300

O	1.07986600	2.26357200	1.28466500
O	2.71520900	2.31740600	-0.13258500
H	-1.52488800	1.14699900	-2.70838100
H	-0.23800700	-0.05571900	-2.60126200
H	-1.64254100	2.77383500	-1.04566100
H	-0.43386600	2.85603700	0.16175900
C	0.97525900	0.79123900	-0.46523400
C	-0.16164800	1.41115600	-1.22374400

IM (for the formation of compound **P3-3**)

C	-0.08501600	0.27893000	0.61829700
O	1.06422400	-0.38962600	0.99925800
C	2.13181500	0.36189200	0.50655400
C	0.46357800	1.51326200	0.00608500
N	1.79924400	1.47139000	-0.05223700
N	-0.97266700	0.53094300	1.86825100
O	-0.37314700	0.95365700	2.82077000
O	-2.16002000	0.33632200	1.75025300
N	-0.33215800	2.61041500	-0.35782600
O	-1.54204900	2.45190900	-0.15321600
O	0.18475100	3.60204200	-0.83164600
N	3.31242800	-0.36208100	0.19967500
O	3.19066800	-1.59130900	0.09609300
O	4.33529800	0.25825900	0.00545000
N	-1.86565600	0.03367500	-1.27767900
N	-1.67580400	-1.82744700	0.36361500
N	0.87113600	-0.82440700	-2.06388400
N	0.62403000	-2.63062200	-0.67357500
O	-3.01196900	0.10823600	-0.96002100
O	-1.33421600	0.55992400	-2.24569600
O	-1.16430000	-2.18184200	1.41251600
O	-2.61115500	-2.33190400	-0.19292200
H	1.73409300	-1.20224300	-2.44156400
H	0.49641500	0.05200900	-2.42336800
H	1.56553800	-2.93119700	-0.91392800
H	0.30522000	-2.95180900	0.23800300
C	-0.91232000	-0.73283500	-0.37102500
C	0.22697500	-1.45210900	-1.11161500

TS2 (for the formation of compound **P3-3**)

C	-0.42743000	-0.20192100	-0.77273800
O	0.80300300	-0.18962600	-1.41687700
C	1.51970500	-0.92948000	-0.47649200
C	-0.42194400	-1.58007500	-0.16862500

N	0.79936900	-1.91663600	0.08124600
N	-1.55292200	0.12965300	-1.72254300
O	-1.50958300	-0.44408700	-2.77896700
O	-2.39196300	0.89425900	-1.30820500
N	-1.59073600	-2.27620000	0.28890100
O	-2.63833700	-1.67496400	0.08426800
O	-1.45304200	-3.35473900	0.81421000
N	2.91840300	-0.85367300	-0.49478100
O	3.42556100	-0.11021500	-1.32748100
O	3.50708200	-1.39008800	0.44134900
N	-1.34505900	0.68076700	1.45140500
N	-0.33625200	2.30957700	-0.12822000
N	1.42570900	0.25483300	2.19743700
N	2.08133100	1.63449400	0.45775600
O	-2.28312000	1.42017800	1.45929500
O	-1.18137100	-0.30062500	2.16305300
O	-0.10552900	2.43845900	-1.31173600
O	-0.50748000	3.17400500	0.68744900
H	2.39480400	0.03030200	2.40559400
H	0.74660000	-0.40300700	2.56312500
H	3.02550900	1.60665500	0.82904100
H	2.04781600	1.80912700	-0.54534400
C	-0.25258300	0.88261100	0.41243000
C	1.19302300	0.74832400	0.96847500

TS1 (for the formation of compound **P3-4**)

C	-1.54363300	-0.36418600	-1.04494400
O	-0.24044100	-0.54724600	-1.49027600
C	0.41997900	0.50218800	-0.92628700
C	-1.56907700	0.87812700	-0.45336200
N	-0.39993400	1.49091900	-0.46980400
N	-2.26400200	-1.50306400	-0.68000700
O	-3.12328300	-1.34825700	0.19717400
O	-1.94069200	-2.57675300	-1.16221200
N	-2.73275600	1.48156200	0.20033900
O	-3.74618600	1.55422600	-0.44939300
O	-2.56220000	1.84570600	1.34925800
N	1.59155900	0.91600100	-1.80093400
O	2.44837400	0.07723600	-1.96497400
O	1.51657500	2.01166800	-2.28869600
N	1.76596500	0.98767800	1.31577800
N	2.37210900	-1.13966600	0.32837100
N	-0.71153600	-0.24201800	2.12989400
N	-0.15464500	-2.19887900	1.08186300

O	2.41417500	1.71254700	0.60345400
O	1.50951000	1.17196700	2.49152000
O	2.08453800	-2.17217500	-0.25669400
O	3.47850600	-0.78933800	0.64903000
H	-1.64134300	-0.59882900	2.32961200
H	-0.52255300	0.72503700	2.36789700
H	-1.00724300	-2.62875200	1.42547300
H	0.36597100	-2.67292000	0.34802100
C	1.22874400	-0.23776700	0.64305900
C	0.10179300	-0.92651600	1.34236100

IM (for the formation of compound **P3-4**)

C	1.56907500	0.18284900	-1.10896600
O	0.22811600	0.28883600	-1.53708800
C	-0.46073300	-0.58425000	-0.70541500
C	1.57739200	-0.91257400	-0.24749400
N	0.42329800	-1.47275400	-0.03933000
N	2.23379800	1.36591700	-0.85308100
O	3.12341700	1.34244600	0.01961300
O	1.87984300	2.38819200	-1.44112700
N	2.75078800	-1.36283500	0.51267400
O	3.71302400	-1.72393900	-0.11276500
O	2.62808000	-1.31802700	1.72519400
N	-1.46834700	-1.32761900	-1.60178900
O	-2.62212600	-0.95833900	-1.57752000
O	-0.97707200	-2.18273900	-2.28669600
N	-1.73589900	-0.71178200	1.51170100
N	-2.44194400	1.03389700	-0.01342200
N	0.68539300	0.79611800	1.92617900
N	-0.06980000	2.41768700	0.48594700
O	-2.19785300	-1.73893700	1.09444800
O	-1.67066200	-0.33808100	2.66433700
O	-2.24452200	1.78607600	-0.94696400
O	-3.46952800	0.84976800	0.57747000
H	1.58781500	1.26037700	2.02314400
H	0.63693500	-0.14765300	2.29918800
H	0.74675000	2.99351500	0.67680800
H	-0.55975500	2.61474400	-0.38572800
C	-1.21750300	0.25417900	0.45574600
C	-0.16464700	1.21755900	1.01499900

TS2 (for the formation of compound **P3-4**)

C	1.24154700	0.25988200	-0.77969200
O	0.12839000	0.09246300	-1.59675100

C	-0.59378400	-0.70697400	-0.70809400
C	1.40374600	-0.99743500	-0.12518000
N	0.30509700	-1.65323700	-0.07365200
N	2.19273000	1.24595000	-1.01695000
O	3.10476600	1.28022500	-0.18082400
O	1.97280900	2.08327200	-1.87511300
N	2.61744500	-1.44516200	0.56920200
O	3.53115800	-1.79326700	-0.13439500
O	2.57565300	-1.40940600	1.78288000
N	-1.69213800	-1.40329100	-1.48468600
O	-2.82602500	-1.01395300	-1.32183600
O	-1.29830600	-2.26887400	-2.22251800
N	-1.58507000	-0.52124100	1.62241900
N	-2.24720500	1.14100800	-0.00527800
N	0.84735100	1.03153100	1.91366500
N	0.06854700	2.49419700	0.31107600
O	-2.10134600	-1.57298000	1.33360100
O	-1.48627500	-0.02387700	2.71931800
O	-2.10327500	1.70071700	-1.06899700
O	-3.19083100	1.19044800	0.73528200
H	1.78088000	1.43880700	1.90151600
H	0.82497100	0.11872400	2.35363600
H	0.78560300	3.13057900	0.64134000
H	-0.23362000	2.64722700	-0.64642800
C	-1.06046700	0.28474100	0.44061000
C	0.14914400	1.21282800	0.76138700

(4) The Cartesian coordinates of TSs and IMs for the reaction between **FOX-7** and **BN7**

TS1 (for the formation of compound **P4-1**)

C	1.18126700	-0.98379900	-0.95043000
O	-0.05419500	-0.81974400	-1.56462600
C	1.61843900	0.22872500	-0.48522000
N	-0.56060400	0.40255700	-1.10987200
C	0.57271900	1.10720800	-0.68310700
N	1.49689800	-2.25336900	-0.46157200
O	0.92665500	-3.22103900	-0.94311600
O	2.27673100	-2.29142500	0.49971300
N	2.85209700	0.47403600	0.25694600
O	3.89086800	0.33658400	-0.33467200
O	2.69538500	0.77681100	1.42516400
N	0.57581700	2.52641900	-0.63141900
O	-0.48078000	3.09928100	-0.82723700
O	1.65519500	3.04184200	-0.38382900
N	-2.73178300	-0.72612300	-0.45306100

N	-1.98481300	1.19366900	0.81429900
N	-0.91759400	-2.30796100	1.01081200
N	0.10951000	-0.49428000	1.97218500
O	-2.98193100	-0.41337600	-1.58075900
O	-3.36485300	-1.49405300	0.25556800
O	-1.16236200	1.76260900	1.51482800
O	-3.08535500	1.58494100	0.52087400
H	-0.22580400	-2.93719100	1.40514200
H	-1.65548200	-2.71415000	0.45158600
H	0.80251400	-1.10733800	2.39167900
H	0.31528200	0.50003200	1.97491800
C	-1.52998400	-0.08356100	0.21234800
C	-0.78178600	-0.99281400	1.12860600

IM (for the formation of compound **P4-1**)

C	1.18419000	-1.00333600	-0.92885500
O	-0.05837800	-0.86713500	-1.57589200
C	1.59474800	0.23743000	-0.48040900
N	-0.60961100	0.34185100	-1.06322200
C	0.55066100	1.09835000	-0.66451400
N	1.51200000	-2.23122100	-0.39138100
O	0.93653300	-3.23476900	-0.81569800
O	2.32544100	-2.23458000	0.54906300
N	2.83544200	0.51908500	0.24125900
O	3.86618700	0.45272200	-0.37387500
O	2.68547300	0.77452000	1.42184800
N	0.54106000	2.50954800	-0.64433500
O	-0.53437700	3.06628500	-0.80770300
O	1.61728500	3.04839400	-0.43359900
N	-2.72855600	-0.73841900	-0.40551000
N	-1.93759700	1.23595500	0.74667400
N	-0.95868300	-2.31388000	0.89810400
N	0.08993700	-0.56870200	1.97750700
O	-2.83990100	-0.90768200	-1.58830800
O	-3.49402200	-1.05429200	0.48016600
O	-1.21618900	1.71640400	1.59911300
O	-2.95222600	1.68916600	0.29986900
H	-0.33147800	-2.98317800	1.33828700
H	-1.37769300	-2.65625400	0.03826100
H	0.80323200	-1.19069800	2.35351300
H	0.25160800	0.43049100	2.07164000
C	-1.45161000	-0.06069400	0.11052700
C	-0.75136100	-1.01710600	1.07071300

TS2 (for the formation of compound **P4-1**)

C	-0.75742700	1.06479400	-0.67560600
O	0.20241200	0.68722900	-1.62076200
C	-1.51358700	-0.08945400	-0.36232400
N	0.57790900	-0.58411000	-1.07714900
C	-0.68772200	-1.11785300	-0.64741800
N	-1.10254800	2.39442500	-0.47852500
O	-0.46432900	3.25551300	-1.06512400
O	-1.92325300	2.58853500	0.42574600
N	-2.81349600	-0.12626600	0.30364400
O	-3.78265600	0.06417600	-0.38210300
O	-2.76982600	-0.32734000	1.50127200
N	-0.99428400	-2.51747000	-0.68896500
O	-0.15492000	-3.27410200	-1.12000900
O	-2.10877700	-2.80123000	-0.27832900
N	2.70817400	0.31724100	-0.63407000
N	1.82669300	-1.23361300	1.01130100
N	1.19221500	2.21205100	1.04522200
N	0.04838000	0.47040500	2.04150400
O	3.35617600	-0.60769200	-1.04219100
O	2.93322200	1.49695100	-0.79284400
O	1.02269400	-2.12781100	1.14656200
O	2.87411100	-1.08504400	1.58280700
H	0.65657700	2.87097000	1.60145700
H	1.67256100	2.59633400	0.23963900
H	-0.50308800	1.15124900	2.55646800
H	-0.44937200	-0.41082200	1.94066500
C	1.41763400	-0.09733500	0.08623900
C	0.71496700	0.95821000	0.95924700

TS1 (for the formation of compound **P4-2**)

C	-1.26490800	-0.39481900	0.54307500
C	-0.18410100	-0.93477300	1.41940800
C	1.08143200	0.67396100	-0.58136100
C	2.00676300	-0.36237000	-0.79720000
O	0.18352200	-1.05400500	-1.65148300
N	1.23421600	1.75970800	0.28152200
O	0.20051300	2.27975800	0.70733000
O	2.36861200	2.07637400	0.60642700
N	3.30469900	-0.50196700	-0.13272500
O	3.20956800	-0.78097900	1.05618900
O	4.31261400	-0.37171700	-0.77000000
N	-2.26749800	-1.38559600	0.08051300
O	-1.82150700	-2.44487800	-0.34306200

O	-3.43255500	-1.08390600	0.12664000
N	-2.00845100	0.77912500	1.10333900
O	-2.01575900	0.91182000	2.31688600
O	-2.55842700	1.48956900	0.30554900
N	0.28926900	-2.14436400	1.18915300
H	-0.12817100	-2.70237800	0.44708300
H	1.17236200	-2.43049500	1.59706100
N	0.43236500	-0.13775400	2.27049000
H	0.04727900	0.77667600	2.48900600
H	1.35901300	-0.37417000	2.61008900
N	1.53950100	-1.38847900	-1.42829400
C	-0.14167500	0.09678700	-1.01322100
N	-1.17819500	0.84120600	-1.83229100
O	-2.12951100	0.17782000	-2.17266500
O	-0.92418200	1.98820400	-2.09298500

IM (for the formation of compound **P4-2**)

C	1.18945200	-0.29678500	-0.41688900
C	0.18561800	-0.85268100	-1.44433400
C	-1.04747800	0.62115500	0.49716700
C	-1.97740400	-0.39551600	0.78292700
O	-0.11037300	-1.18090300	1.47695200
N	-1.25625900	1.67586500	-0.35647000
O	-0.24351900	2.21541800	-0.84997500
O	-2.40447700	1.99235800	-0.64232500
N	-3.31067100	-0.48772300	0.17783300
O	-3.26781600	-0.78791800	-1.00782200
O	-4.28760100	-0.30176800	0.84916300
N	2.29110800	-1.32806700	-0.08658800
O	1.91168700	-2.44011600	0.21639700
O	3.42662200	-0.94789700	-0.16201400
N	1.98636900	0.89040600	-0.95133600
O	2.20454900	0.86950300	-2.14667300
O	2.38547700	1.68065600	-0.14610800
N	-0.28275800	-2.06217900	-1.23515100
H	0.06017200	-2.60039100	-0.44152300
H	-1.13147600	-2.36885300	-1.70017800
N	-0.28229600	-0.08998500	-2.40529700
H	0.01780000	0.88121500	-2.47821400
H	-1.13241100	-0.35824200	-2.89122100
N	-1.51010100	-1.45130100	1.34731000
C	0.24606200	0.02375700	0.85166300
N	1.11194500	0.76382500	1.90235300
O	2.12455900	0.16835900	2.20398000

O	0.68302500	1.79115800	2.35084500

TS2 (for the formation of compound **P4-2**)

C	-0.30834100	0.60350800	-0.65720100
O	-0.11242500	-0.09593100	-1.84356500
C	1.09698100	0.76416000	-0.14048800
N	0.82772400	-1.09723600	-1.40733500
C	1.67040200	-0.35791400	-0.61570700
N	-1.06504300	1.88634700	-0.91495100
O	-0.67258800	2.52766300	-1.85310800
O	-1.96390900	2.14403300	-0.14598300
N	1.64676800	1.82175700	0.64754200
O	2.70743200	1.58888400	1.19846800
O	1.01193500	2.85677600	0.68696600
N	2.97783900	-0.93599800	-0.31711800
O	2.94401300	-2.03622100	0.20798300
O	3.94996700	-0.30514900	-0.63692900
N	-2.58025200	-0.39763800	-0.10877100
N	-0.98659800	-0.15382600	1.72081300
N	-1.28690500	-2.58833400	-0.98803300
N	0.15899500	-2.54351500	0.81734900
O	-3.36667400	-0.40426700	0.79509600
O	-2.81701000	-0.34464600	-1.29769200
O	-0.55736800	0.93815900	2.02194100
O	-1.36038500	-1.02344300	2.46946400
H	-0.94590600	-3.52348200	-1.17866000
H	-1.60769000	-2.09626100	-1.81651700
H	0.70586800	-3.32595900	0.47291800
H	0.67690200	-2.01564200	1.50914000
C	-1.08386900	-0.44847200	0.23333400
C	-0.50530300	-1.85235300	-0.14568500

TS1 (for the formation of compound **P4-3**)

C	0.12573600	0.31883500	-0.83500100
O	-0.14929900	-0.65689800	-1.73480100
C	-1.10247600	0.65182700	-0.21082800
N	-1.46750100	-1.15609800	-1.53933400
C	-1.97667900	-0.34368000	-0.67215900
N	0.98634800	1.42816400	-1.45703300
O	1.98641600	1.77315200	-0.87704900
O	0.52368800	1.86781900	-2.47695800
N	-1.37103100	1.77046000	0.59409300
O	-2.50633400	1.88721700	1.02733900
O	-0.43739300	2.54036100	0.78418400

N	-3.29196600	-0.66437500	-0.11184600
O	-4.26498200	-0.47704300	-0.79485900
O	-3.25015400	-1.13150600	1.01280100
N	1.34608300	0.38576100	1.62581100
N	2.70454500	-0.64426000	-0.17101900
N	-0.32191700	-1.99648100	1.37108500
N	1.10797200	-2.80243500	-0.23321000
O	2.24411400	1.15930500	1.79662200
O	0.34418900	0.29337600	2.33575100
O	2.70192300	-0.90172600	-1.37061000
O	3.67012200	-0.59593900	0.53975300
H	-0.89422000	-2.83071300	1.32296500
H	-0.62263000	-1.22482200	1.96392400
H	0.57808800	-3.66343700	-0.28083900
H	1.70989300	-2.58579800	-1.02343300
C	1.33898100	-0.47535300	0.41517300
C	0.69490700	-1.81918400	0.55784800

IM (for the formation of compound **P4-3**)

C	0.19421700	-0.25423400	0.72020100
O	-0.11101200	0.71312700	1.66907800
C	-1.08223400	-0.55835200	0.08807300
N	-1.47102400	1.16579600	1.53267700
C	-1.96927500	0.36814500	0.65241600
N	0.86834800	-1.46879100	1.42553000
O	1.95591700	-1.81705800	1.02529700
O	0.20872300	-1.94914400	2.30635900
N	-1.35882400	-1.70258600	-0.64585500
O	-2.51086600	-1.88992600	-1.01389300
O	-0.39904700	-2.44317000	-0.87808000
N	-3.30009800	0.68022800	0.12133200
O	-4.26249000	0.48707100	0.81644000
O	-3.27852000	1.15848600	-1.00110500
N	1.39715800	-0.44611700	-1.58128500
N	2.67361200	0.59400200	0.28092400
N	-0.28469700	1.98296300	-1.35393700
N	1.23574500	2.80222200	0.16152200
O	2.27212800	-1.25421000	-1.64267900
O	0.53356500	-0.23730700	-2.41841100
O	2.69362500	0.80337300	1.48102700
O	3.59912500	0.65862600	-0.48152700
H	-0.81099700	2.84982400	-1.36390200
H	-0.64470800	1.19268800	-1.88777500
H	0.80354800	3.71799100	0.12784300

H	1.80461000	2.59889600	0.98022100
C	1.28380000	0.39525200	-0.30526000
C	0.72629400	1.80713100	-0.54589500

TS2 (for the formation of compound **P4-3**)

C	0.36000000	0.57488100	-0.72156800
O	0.17630700	-0.21608600	-1.85492600
C	-1.06378000	0.83356600	-0.30199700
N	-0.80762800	-1.15129600	-1.36499400
C	-1.65966700	-0.30746100	-0.68263000
N	1.17178500	1.81089600	-1.02595700
O	1.95639300	2.14875600	-0.17182600
O	0.91052400	2.35261000	-2.06896100
N	-1.53032900	1.84442000	0.58556100
O	-2.70816000	1.82172000	0.88051900
O	-0.68554400	2.63173800	0.97841600
N	-2.98233900	-0.81705300	-0.33475100
O	-3.92983600	-0.28832800	-0.85259800
O	-2.98045300	-1.76417000	0.43072000
N	0.84627200	0.02798100	1.70982700
N	2.53867400	-0.58182300	0.00639700
N	-0.19669900	-2.52240200	0.93277700
N	1.24390100	-2.60188200	-0.87352400
O	1.75015700	0.57691500	2.26971600
O	-0.28575600	-0.13791200	2.14184700
O	2.90185000	-0.26260400	-1.10712300
O	3.18921000	-1.09963100	0.87193400
H	-0.53463400	-3.44534700	0.68636700
H	-0.85076400	-1.99938000	1.50313600
H	0.88383700	-3.52860200	-1.07200900
H	1.54562200	-2.12739200	-1.72056700
C	1.04739200	-0.43398300	0.27832700
C	0.41821300	-1.84454200	-0.06980600

TS1 (for the formation of compound **P4-4**)

C	1.20384000	1.00098000	-0.90081300
O	-0.00958700	0.88784800	-1.56467300
C	1.59946100	-0.24055600	-0.46938800
N	-0.56460300	-0.33811300	-1.17829800
C	0.55409100	-1.08666500	-0.75804400
N	1.56185200	2.24202500	-0.38660100
O	0.99536300	3.24099300	-0.82120000
O	2.38123500	2.23694800	0.54030500
N	2.79956400	-0.54442800	0.30620500

O	2.59691300	-0.77318500	1.48312000
O	3.85382600	-0.52079600	-0.27246000
N	0.53009200	-2.50397900	-0.70090400
O	-0.53186100	-3.05877100	-0.92146100
O	1.59350900	-3.03764700	-0.42672300
N	-1.86893200	-1.24590000	0.75734200
N	-2.78308600	0.71127400	-0.35462500
N	0.01020500	0.66321500	2.01296300
N	-1.03718600	2.33714200	0.80610000
O	-2.85094600	-1.78837400	0.32800000
O	-1.05516200	-1.71197000	1.54508200
O	-2.73756000	1.17391300	-1.47049100
O	-3.69571600	0.77241000	0.43443000
H	0.69644900	1.31634500	2.38027600
H	0.17322400	-0.32843200	2.16603900
H	-0.44156200	3.03875700	1.23574700
H	-1.40832000	2.61301700	-0.10028100
C	-1.51902600	0.07081600	0.17948700
C	-0.81757500	1.04554200	1.05734400

IM (for the formation of compound **P4-4**)

C	-1.18420200	-1.00334300	-0.92881900
O	0.05835100	-0.86717400	-1.57588500
C	-1.59473700	0.23743600	-0.48039400
N	0.60961300	0.34182000	-1.06326400
C	-0.55064800	1.09834200	-0.66455600
N	-1.51205500	-2.23121800	-0.39135500
O	-0.93659300	-3.23478100	-0.81565500
O	-2.32553300	-2.23455800	0.54905300
N	-2.83540800	0.51912800	0.24129700
O	-2.68541000	0.77451200	1.42189400
O	-3.86616300	0.45284600	-0.37382700
N	-0.54104300	2.50953800	-0.64437600
O	0.53438800	3.06627600	-0.80778000
O	-1.61726200	3.04838400	-0.43360500
N	1.93756100	1.23597500	0.74663600
N	2.72857900	-0.73842400	-0.40546000
N	-0.08986600	-0.56876200	1.97754400
N	0.95872000	-2.31388800	0.89799700
O	2.95215100	1.68923200	0.29979200
O	1.21616000	1.71639900	1.59909800
O	2.83983400	-0.90800200	-1.58822600
O	3.49412500	-1.05402300	0.48023700
H	-0.80313600	-1.19077500	2.35356500

H	-0.25152000	0.43042800	2.07173700
H	0.33158900	-2.98322200	1.33822900
H	1.37755300	-2.65620400	0.03804000
C	1.45161000	-0.06069300	0.11050800
C	0.75138000	-1.01712400	1.07068300

TS2 (for the formation of compound **P4-4**)

C	0.89564800	1.03177200	-0.65456300
O	-0.10345100	0.84193400	-1.61000200
C	1.48994700	-0.22922600	-0.40261200
N	-0.64251900	-0.40231400	-1.16611800
C	0.55470100	-1.11985500	-0.78721500
N	1.44287700	2.29076700	-0.44334100
O	0.93023800	3.24601300	-1.01375800
O	2.30651800	2.34889900	0.43669700
N	2.72772800	-0.47485300	0.33046700
O	2.58094500	-0.59040600	1.53102200
O	3.74774200	-0.52039200	-0.30347000
N	0.59238000	-2.54372500	-0.72450900
O	-0.44656100	-3.13470900	-0.94867800
O	1.67202200	-3.02620400	-0.43231300
N	-1.68510900	-1.27608900	0.82798400
N	-2.74298300	0.58547600	-0.33144300
N	-0.06475600	0.84251300	2.07216400
N	-1.12223100	2.36675400	0.67749500
O	-2.70604600	-1.83563200	0.54241700
O	-0.80852800	-1.67306100	1.57440900
O	-2.88004400	0.89823700	-1.48691900
O	-3.52031400	0.72009500	0.58109600
H	0.50096100	1.58727800	2.46786800
H	0.32032200	-0.08682700	2.20692600
H	-0.66306700	3.11983600	1.18021100
H	-1.34331500	2.62134900	-0.28338500
C	-1.38121900	0.01320900	0.08376100
C	-0.64787200	1.11084500	0.88821000

(5) The Cartesian coordinates of TSs and IMs for the reaction between **FOX-7** and **DN3**

TS1 (for the formation of compound **P5-1**)

C	-1.14674000	-1.19748500	-0.56444500
O	-0.75937400	-0.28222400	-1.54380900
N	0.55972500	-0.02029500	-1.10157000
N	-0.14122200	-1.98000400	-0.17535100
C	0.89511600	-1.30675000	-0.56809200
N	-2.49230100	-1.33270500	-0.23307500

O	-2.74978900	-2.00959000	0.76428900
O	-3.29008800	-0.62089900	-0.83382800
N	2.26158400	-1.73846400	-0.39931900
O	3.08351600	-1.26011700	-1.15052200
O	2.45793900	-2.54539300	0.49075300
N	-0.25022100	2.19398800	-0.72919100
N	1.49389100	1.40885000	0.76395200
N	-1.96026000	0.90015700	1.31909100
N	-0.14243600	-0.30375200	2.09600100
O	0.61351200	2.71415500	-1.38123400
O	-1.42406500	2.49894900	-0.69412400
O	2.32199300	0.53616200	0.91276200
O	1.53264600	2.54042600	1.16903300
H	-2.57549100	0.34611600	1.90895400
H	-2.40339000	1.40900200	0.56142600
H	-0.77162200	-0.85654300	2.67148500
H	0.73283300	-0.77992800	1.89208500
C	0.21543300	0.98419700	0.06988600
C	-0.72613600	0.42256600	1.11527300

TS1 (for the formation of compound **P5-2**)

C	0.07845600	0.88702500	-0.07809100
O	0.44059800	0.91011400	-1.39996300
N	1.80715200	0.53162400	-1.44981900
N	1.15174700	0.73750800	0.73399500
C	2.09161900	0.48363800	-0.18703300
N	-0.80951700	2.08192200	0.29968400
O	-1.52856300	1.92819600	1.26115800
O	-0.63626500	3.07935700	-0.34775000
N	3.41724700	-0.00467100	0.20752400
O	4.37761200	0.40251600	-0.39904900
O	3.41763100	-0.83289900	1.10472600
N	-2.10221900	-0.35921300	-1.04863800
N	-1.77032000	-0.62724200	1.32560000
N	-0.13888600	-2.39175100	-1.34100700
N	0.71817900	-1.98131900	0.75299300
O	-2.44704300	0.77500700	-1.25150600
O	-2.54885300	-1.35141600	-1.60383900
O	-1.06308100	-0.77413800	2.30134900
O	-2.97353700	-0.53900900	1.30232800
H	0.59571800	-3.05682300	-1.54284400
H	-0.90531700	-2.28828500	-1.99547400
H	1.45375600	-2.66696400	0.62771200
H	0.82324100	-1.32073600	1.52463500

C	-1.05292000	-0.54423500	0.01270700
C	-0.14867000	-1.71926600	-0.20024800

IM (for the formation of compound **P5-2**)

C	0.07511000	0.76783300	-0.08232600
O	0.45635800	0.80139900	-1.41498300
N	1.85161900	0.48630000	-1.46329200
N	1.17394900	0.57264600	0.72917800
C	2.11878900	0.40264900	-0.20129000
N	-0.65634800	2.08646000	0.30732000
O	-1.47858900	1.99597900	1.19572400
O	-0.26920300	3.07765500	-0.24664400
N	3.44279700	-0.09543600	0.18944700
O	4.41834500	0.39263800	-0.32431600
O	3.42392200	-1.02032100	0.98851000
N	-2.14388700	-0.19152600	-1.01852100
N	-1.76351200	-0.53760800	1.35568700
N	-0.48905800	-2.46646100	-1.32489900
N	0.63034800	-2.04183900	0.64116700
O	-2.33205000	0.95152900	-1.33159700
O	-2.77241800	-1.16037800	-1.41390400
O	-1.03819600	-0.72541000	2.30378300
O	-2.96293700	-0.43027400	1.34606100
H	0.12042100	-3.24466700	-1.54162200
H	-1.30560200	-2.30491900	-1.90341300
H	1.26089500	-2.82373500	0.50128200
H	0.91745500	-1.31938600	1.31691900
C	-1.05268900	-0.44321300	0.00819700
C	-0.28727300	-1.73686700	-0.24239000

TS2 (for the formation of compound **P5-2**)

C	-0.23416000	0.98552700	-0.09354800
O	0.10025100	0.98295500	-1.44215300
N	1.27742500	0.14686100	-1.35333800
N	0.97754500	1.18086300	0.66363800
C	1.78247000	0.64846200	-0.17167300
N	-1.29427700	2.00850300	0.22304600
O	-1.54082300	2.14007600	1.39696500
O	-1.80384400	2.55766200	-0.72447400
N	3.20212900	0.41197200	0.15110200
O	4.00744000	0.88506600	-0.61275600
O	3.42293300	-0.24856700	1.14816300
N	-2.12884900	-0.48250400	-0.65135900
N	-1.01927700	-1.04033700	1.43657300

N	0.01311300	-2.16688300	-1.67643000
N	1.14556800	-1.99467400	0.32664700
O	-3.04155200	-0.13450500	0.05719000
O	-2.18206000	-0.71080800	-1.83824500
O	-0.41073200	-0.51649000	2.33873100
O	-1.74339200	-2.00334000	1.48893300
H	0.79114400	-2.69030800	-2.06141900
H	-0.54682400	-1.70691100	-2.38377400
H	1.79779400	-2.69059300	-0.01175000
H	1.49387800	-1.45508400	1.11528800
C	-0.76621900	-0.50336000	0.04106400
C	0.34867300	-1.38398300	-0.60856400

TS1 (for the formation of compound **P5-3**)

C	-0.07844100	0.88700700	-0.07808900
O	-0.44058800	0.91010200	-1.39996200
N	-1.80714800	0.53162900	-1.44981500
N	-1.15173800	0.73750200	0.73399800
C	-2.09161200	0.48364400	-0.18702900
N	0.80952100	2.08192000	0.29968100
O	1.52859700	1.92820000	1.26113300
O	0.63622800	3.07935800	-0.34773700
N	-3.41724100	-0.00466300	0.20752500
O	-4.37759900	0.40247000	-0.39909500
O	-3.41763100	-0.83284200	1.10477300
N	1.77032000	-0.62724200	1.32559600
N	2.10220900	-0.35921200	-1.04864500
N	-0.71817300	-1.98131900	0.75301400
N	0.13886600	-2.39175100	-1.34099700
O	2.97353900	-0.53905400	1.30231100
O	1.06308300	-0.77410200	2.30135100
O	2.44704500	0.77500600	-1.25150000
O	2.54882700	-1.35141300	-1.60386000
H	-1.45375600	-2.66696000	0.62774600
H	-0.82321300	-1.32074000	1.52466400
H	-0.59573700	-3.05682700	-1.54282700
H	0.90528500	-2.28827400	-1.99547700
C	1.05291000	-0.54422700	0.01270500
C	0.14865900	-1.71926600	-0.20024000

IM (for the formation of compound **P5-3**)

C	-0.07511000	0.76783300	-0.08232600
O	-0.45635800	0.80139900	-1.41498300
N	-1.85161900	0.48630000	-1.46329200

N	-1.17394900	0.57264600	0.72917800
C	-2.11878900	0.40264900	-0.20129000
N	0.65634800	2.08646000	0.30732000
O	1.47858900	1.99597900	1.19572400
O	0.26920300	3.07765500	-0.24664400
N	-3.44279700	-0.09543600	0.18944700
O	-4.41834500	0.39263800	-0.32431600
O	-3.42392200	-1.02032100	0.98851000
N	1.76351200	-0.53760800	1.35568700
N	2.14388700	-0.19152600	-1.01852100
N	-0.63034800	-2.04183900	0.64116700
N	0.48905800	-2.46646100	-1.32489900
O	2.96293700	-0.43027400	1.34606100
O	1.03819600	-0.72541000	2.30378300
O	2.33205000	0.95152900	-1.33159700
O	2.77241800	-1.16037800	-1.41390400
H	-1.26089500	-2.82373500	0.50128200
H	-0.91745500	-1.31938600	1.31691900
H	-0.12042200	-3.24466700	-1.54162200
H	1.30560200	-2.30491900	-1.90341300
C	1.05268900	-0.44321300	0.00819700
C	0.28727300	-1.73686700	-0.24239000

TS2 (for the formation of compound **P5-3**)

C	0.29955600	1.00593700	-0.23008600
O	-0.03442400	0.91124400	-1.56828600
N	-1.24507200	0.13589100	-1.42834100
N	-0.89900100	1.33237700	0.49384400
C	-1.71625200	0.70824200	-0.27090000
N	1.39028200	2.00826200	0.02338100
O	1.93616500	1.88082500	1.09707200
O	1.57159000	2.84359100	-0.82163900
N	-3.09933800	0.42486900	0.12325200
O	-3.45798200	-0.72114200	-0.08861700
O	-3.73471300	1.31491100	0.62583400
N	0.51786000	-0.74939300	1.63686400
N	2.14348200	-0.81392100	-0.20133300
N	-0.96006000	-2.36340700	-0.23753800
N	0.47504100	-1.74605100	-1.93947200
O	1.48305800	-0.64267300	2.34086900
O	-0.62451000	-0.97324700	1.99851300
O	2.66663200	-0.04864700	-0.98626700
O	2.59688300	-1.83082200	0.24886800
H	-1.49815900	-2.90440600	-0.90422500

H	-1.48188400	-2.11263900	0.59306100
H	-0.07285400	-2.32250600	-2.56818100
H	0.91154400	-0.96555700	-2.42245900
C	0.69956700	-0.50351600	0.15227200
C	-0.17330500	-1.40526300	-0.77854800

TS1 (for the formation of compound **P5-4**)

C	-0.31218300	1.06903100	0.07306900
C	0.91965400	0.79282900	0.79248000
O	0.81423500	-0.41803900	-1.46240500
N	-0.39189600	2.17069300	-0.90092300
O	0.62126500	2.40352400	-1.53603900
O	-1.46511400	2.70757000	-1.03227800
N	-1.50980500	1.12873600	0.96787300
O	-2.34683100	0.26560400	0.87202600
O	-1.51200600	2.07491100	1.72133900
N	2.05604100	1.52401800	0.55875800
H	2.21692400	1.87567500	-0.37875200
H	2.87798800	1.22683900	1.07276700
N	0.69418000	0.26465400	2.08940500
H	1.40492800	-0.41921700	2.34551300
H	0.65687100	1.01555800	2.77748900
N	0.29416500	-1.84255000	0.19785900
N	-0.55068300	-0.32223800	-1.25049100
C	-0.75958600	-1.42479900	-0.42637400
C	1.20906600	-0.97298100	-0.28179100
N	-2.08585700	-2.03397300	-0.29713300
O	-2.89603200	-1.70816100	-1.13494500
O	-2.22165300	-2.81874800	0.61113500
N	2.63133800	-1.15963800	-0.10049600
O	2.97010400	-1.54892900	1.00489000
O	3.35343300	-0.78163700	-0.99563100

(6) The Cartesian coordinates of TSs and IMs for the reaction between **FOX-7** and **FN2**

TS1 (for the formation of compounds **P6-1 and P6-2**)

O	1.00476200	0.83468800	0.61369600
N	1.73298000	0.82171000	-1.48980800
N	-1.70673400	-0.89649300	-1.31478400
N	-2.02346700	-0.44859400	1.09620800
N	0.88022400	-2.04469400	-0.47624000
N	0.31191200	-1.67951700	1.71005800
O	-2.79943500	-0.44084700	-1.49831300
O	-1.05736000	-1.54557200	-2.12233700
O	-1.62783500	0.22067700	2.04370400

O	-3.06360300	-1.04238400	1.02575800
H	1.75363800	-2.47199800	-0.18403700
H	0.65497300	-1.94105400	-1.46358800
H	1.24438100	-1.98143500	1.98011800
H	-0.15569200	-1.06529100	2.37173300
C	-1.01909000	-0.57232900	-0.01609500
C	-0.05016900	0.88434400	-0.24916500
C	2.08641200	0.75921800	-0.24245700
C	0.07441800	-1.52408400	0.41941200
N	0.40838500	0.95042700	-1.55924900
N	3.21905100	0.03083900	0.19970900
O	3.04131100	-0.73625700	1.15833400
O	4.25756600	0.15070300	-0.41213500
N	-0.99209100	2.03966200	0.12402800
O	-0.45701400	3.00713200	0.59688300
O	-2.15571000	1.89729600	-0.18107400

IM1 (for the formation of compounds **P6-1 and P6-2**)

O	-0.99010000	0.72489900	-0.70396300
N	-1.72838700	0.90178700	1.39312400
N	1.74938000	-0.74336100	1.32665600
N	2.01566600	-0.48942200	-1.07298400
N	-0.85809200	-1.88655400	0.78115500
N	-0.29661700	-1.99833100	-1.44256000
O	2.34727600	0.18893500	1.78046600
O	1.70820800	-1.88418600	1.74757400
O	1.57766200	-0.17145200	-2.16706200
O	3.13734600	-0.81316300	-0.79997800
H	-1.73202000	-2.37761500	0.61616700
H	-0.68082100	-1.50743300	1.70836400
H	-1.19946600	-2.41709100	-1.64968400
H	0.17095100	-1.53089200	-2.21583000
C	0.98117600	-0.48475100	0.03610000
C	0.08608000	0.82951300	0.15421100
C	-2.08807500	0.78293000	0.14770200
C	-0.08566500	-1.55506400	-0.22411600
N	-0.41151400	0.94169500	1.49229700
N	-3.20649600	-0.01205300	-0.20622600
O	-3.01434200	-0.88988100	-1.06408700
O	-4.25315200	0.16533500	0.38044500
N	0.90465500	2.07971100	-0.27991100
O	0.24182900	3.07176400	-0.43022100
O	2.10778500	1.96312000	-0.37858100

TS2 (for the formation of compounds **P6-1 and P6-2**)

O	0.69037900	-1.37221600	-0.38053800
N	1.25697400	-0.72599900	1.71002400
N	-1.57228900	1.25807600	0.93655100
N	-1.35361900	0.63423700	-1.42519500
N	1.15846900	2.16670800	0.60434000
N	1.18421300	1.22407800	-1.51409200
O	-2.72305900	1.41278500	0.63662900
O	-1.04457100	1.56028700	1.99033000
O	-1.42177100	-0.40388400	-2.04900200
O	-1.69420800	1.73095500	-1.78025100
H	2.14668600	2.39402500	0.53525600
H	0.79158800	2.13359700	1.54951600
H	2.09419100	1.64690200	-1.66953900
H	1.04642800	0.37617300	-2.06138700
C	-0.66370400	0.55955900	-0.06444200
C	-0.40102900	-0.98927200	0.35967700
C	1.62983700	-0.72524900	0.40915800
C	0.71285700	1.22693800	-0.24494200
N	0.00563500	-0.97075500	1.76244100
N	2.90598900	-0.46984200	-0.08799200
O	3.13595800	-0.80928100	-1.24515700
O	3.63441300	0.23640900	0.60887500
N	-1.59397200	-1.86349200	0.14581700
O	-1.40526700	-2.95674700	-0.31398300
O	-2.63268200	-1.36751100	0.52887100

IM2 (for the formation of compounds **P6-1 and P6-2**)

C	0.81292700	-1.06544800	0.10539700
C	-0.71212200	-0.50776800	0.03599500
C	-0.42916900	0.97817800	-0.27424600
C	1.49138000	0.31783600	-0.20550200
N	0.08232600	1.03049700	-1.71238400
N	1.24294700	0.62968800	-1.65200600
O	0.71394200	1.25651000	0.46049800
N	-1.57147700	-1.19304000	-0.98647700
O	-2.15938000	-0.47965200	-1.76526700
O	-1.61242300	-2.40093300	-0.91688800
N	-1.42350600	-0.63839600	1.37744400
O	-0.97220400	0.06299500	2.25940600
O	-2.33662400	-1.41451000	1.46451100
N	2.92516400	0.35964100	0.16059300
O	3.61456000	-0.40235900	-0.48540600
O	3.25755000	1.10064100	1.05000600

N	-1.50969600	1.97682500	-0.03116100
O	-1.19135600	3.12340200	-0.22157900
O	-2.58627700	1.53566000	0.30719000
N	1.05409200	-1.96749000	-0.97363800
H	2.05968100	-2.10684800	-1.06364300
H	0.58535300	-2.85854000	-0.83399000
N	1.27666500	-1.49932300	1.38347600
H	1.04409100	-0.86894700	2.14812300
H	0.97487900	-2.44529800	1.59894900

TS3 (for the formation of compounds **P6-1 and P6-2**)

C	-0.74049500	-1.08516700	-0.19491100
C	0.75189300	-0.44446100	-0.05102600
C	0.44019100	0.99335700	0.24302000
C	-1.52098400	0.22403800	0.05469000
N	-0.29933100	0.78750200	2.15816800
N	-1.34896100	0.38318200	1.96430800
O	-0.78314500	1.27230800	-0.22647700
N	1.60035300	-1.16144500	0.96675000
O	2.11204800	-0.50050100	1.83464700
O	1.69628700	-2.35943300	0.79690300
N	1.50276300	-0.51713900	-1.39288400
O	1.02371100	0.20768800	-2.24573000
O	2.44027100	-1.25417700	-1.51048000
N	-2.93129700	0.31125900	-0.28269200
O	-3.58077800	-0.65039300	0.08364300
O	-3.32541800	1.30822500	-0.84039600
N	1.42007300	2.03256900	0.02164600
O	1.02483500	3.17568200	0.01243300
O	2.56664800	1.63544600	-0.09891000
N	-0.97994800	-2.02384100	0.85741800
H	-1.97991100	-2.22084900	0.87932400
H	-0.45692200	-2.88304000	0.70985700
N	-1.10062200	-1.56291200	-1.49586500
H	-0.84134700	-0.94603000	-2.26185500
H	-0.74234100	-2.49967100	-1.66096200

1,3-Diradical + N_2 (for the formation of compounds **P6-1 and P6-2**)

C	-0.73311800	-1.11950300	-0.29433200
C	0.75737100	-0.46593800	-0.12466800
C	0.46833300	0.96311600	0.09163300
C	-1.52292900	0.17626200	-0.22803200
N	-0.40921900	0.75634300	2.56767300
N	-1.42814500	0.38321400	2.37262100

O	-0.80121900	1.22997800	-0.15092800
N	1.57843500	-1.17490500	0.93152600
O	2.06447500	-0.51127400	1.81015300
O	1.67054700	-2.37627500	0.77478000
N	1.52153000	-0.57604900	-1.45200200
O	1.02975300	0.12285000	-2.32136900
O	2.46194200	-1.30978500	-1.55060000
N	-2.93994800	0.30833400	-0.35124200
O	-3.57093100	-0.66782400	0.02469600
O	-3.37907100	1.34337600	-0.80312800
N	1.40772000	2.01238300	-0.02944700
O	1.00716700	3.15823800	-0.00587100
O	2.56617800	1.62862200	-0.13157800
N	-1.00478000	-1.95391900	0.84401100
H	-2.00654800	-2.13951800	0.86218500
H	-0.48797500	-2.82773600	0.77558800
N	-1.04250200	-1.72951100	-1.54982100
H	-0.78083700	-1.17481600	-2.36120200
H	-0.65193500	-2.66587500	-1.62062700

TS1 (for the formation of compounds **P6-3 and P6-4**)

C	-1.01906600	-0.57221800	0.01613200
C	0.07444300	-1.52414800	-0.41906000
C	2.08641900	0.75920200	0.24240400
C	-0.05018100	0.88432700	0.24913900
N	1.73300100	0.82176800	1.48975900
N	0.40841700	0.95047300	1.55923100
O	1.00474300	0.83462500	-0.61373700
N	-1.70701000	-0.89626600	1.31469700
O	-1.05768300	-1.54496800	2.12259000
O	-2.79990000	-0.44090400	1.49782100
N	-2.02320700	-0.44862600	-1.09642400
O	-1.62744800	0.22070500	-2.04381400
O	-3.06322000	-1.04266700	-1.02624400
N	3.21903500	0.03079500	-0.19974900
O	3.04132300	-0.73619000	-1.15846100
O	4.25752500	0.15054900	0.41216900
N	-0.99206600	2.03967900	-0.12405700
O	-2.15569600	1.89730200	0.18101300
O	-0.45698000	3.00715600	-0.59687900
N	0.87998900	-2.04471100	0.47684200
H	1.75318500	-2.47263400	0.18492800
H	0.65454300	-1.94084100	1.46413100
N	0.31211400	-1.67982600	-1.70964600

H	1.24464900	-1.98175000	-1.97949100
H	-0.15527800	-1.06561700	-2.37148600

IM1 (for the formation of compounds **P6-3 and P6-4**)

C	-0.98117600	-0.48475300	0.03610000
C	0.08566600	-1.55506300	-0.22412100
C	2.08807400	0.78293100	0.14770300
C	-0.08608100	0.82951300	0.15421100
N	1.72838500	0.90178600	1.39312600
N	0.41151300	0.94169400	1.49229800
O	0.99010000	0.72490100	-0.70396300
N	-1.74937700	-0.74336400	1.32665700
O	-1.70819600	-1.88418800	1.74758000
O	-2.34727800	0.18892900	1.78046500
N	-2.01566800	-0.48942300	-1.07298200
O	-1.57766800	-0.17144800	-2.16706000
O	-3.13734700	-0.81316700	-0.79997500
N	3.20649600	-0.01205200	-0.20622500
O	3.01434200	-0.88987800	-1.06408800
O	4.25315200	0.16533600	0.38044700
N	-0.90465700	2.07971000	-0.27991000
O	-2.10778700	1.96311900	-0.37857700
O	-0.24183100	3.07176300	-0.43022100
N	0.85809500	-1.88655600	0.78114700
H	1.73202500	-2.37761200	0.61615400
H	0.68082100	-1.50744600	1.70835900
N	0.29661800	-1.99832400	-1.44256800
H	1.19946700	-2.41708200	-1.64969400
H	-0.17095000	-1.53088100	-2.21583600

TS2 (for the formation of compounds **P6-3 and P6-4**)

C	0.66372200	-0.55955900	0.06447200
C	-0.71287900	-1.22683500	0.24514000
C	-1.62979200	0.72510600	-0.40915300
C	0.40104200	0.98924100	-0.35970400
N	-1.25694500	0.72584500	-1.71005300
N	-0.00562600	0.97061800	-1.76248000
O	-0.69038100	1.37223500	0.38046100
N	1.57216800	-1.25814900	-0.93661200
O	1.04427300	-1.56051700	-1.99025900
O	2.72300700	-1.41274200	-0.63689700
N	1.35376300	-0.63417100	1.42515000
O	1.42170200	0.40393300	2.04902000
O	1.69463800	-1.73082200	1.78012600

N	-2.90599900	0.46980500	0.08795800
O	-3.13602300	0.80935100	1.24507400
O	-3.63440200	-0.23645400	-0.60891600
N	1.59395500	1.86351000	-0.14589200
O	2.63271500	1.36750500	-0.52877000
O	1.40517400	2.95684000	0.31370500
N	-1.15858600	-2.16677300	-0.60393700
H	-2.14683800	-2.39392200	-0.53476900
H	-0.79181800	-2.13377400	-1.54916100
N	-1.18406800	-1.22385000	1.51436700
H	-2.09406400	-1.64657800	1.66996700
H	-1.04611400	-0.37593500	2.06159600

IM2 (for the formation of compounds **P6-3 and P6-4**)

C	0.70573300	-0.50967200	0.03777900
C	-0.78446300	-1.07112100	-0.00116000
C	-1.46476400	0.33438600	-0.18697000
C	0.45397900	0.98936200	-0.23692500
N	-1.23281100	0.73347200	-1.62506200
N	-0.06752100	1.11884300	-1.66889700
O	-0.68365400	1.23205400	0.51711500
N	1.59304200	-1.19454500	-0.97337100
O	2.10432400	-0.48575400	-1.80624500
O	1.68916000	-2.39648000	-0.87009200
N	1.30908000	-0.69047100	1.43579200
O	1.34307000	0.28993100	2.13507800
O	1.65339400	-1.81154800	1.72724800
N	-2.89790700	0.39796000	0.18721300
O	-3.29337100	1.37686200	0.75842300
O	-3.54469900	-0.57482900	-0.16934900
N	1.54700800	1.97335700	0.01343500
O	2.66967900	1.52714000	0.07087100
O	1.18763600	3.12205500	0.07977500
N	-0.98786000	-1.86368300	-1.18250000
H	-0.58128100	-2.78958800	-1.07113700
H	-1.98641300	-1.94939000	-1.36406900
N	-1.15147400	-1.57405800	1.29810800
H	-2.11787200	-1.89540400	1.26629200
H	-0.56257000	-2.36490600	1.55694100

TS3 (for the formation of compounds **P6-3 and P6-4**)

C	-0.73291600	-0.46769300	-0.03485100
C	0.74236300	-1.08731400	-0.01885800
C	1.50635000	0.25153700	0.05146700

C	-0.46100400	1.00146400	0.12013400
N	1.28363400	0.66758400	1.93799400
N	0.21378800	1.06245000	2.02325100
O	0.75464400	1.24830000	-0.36759900
N	-1.62435900	-1.07328900	1.02605500
O	-2.16174300	-0.31061000	1.79021900
O	-1.70876400	-2.28180200	1.01045400
N	-1.39051600	-0.72077400	-1.41742800
O	-1.28035400	0.18313600	-2.20661000
O	-1.88840300	-1.80354700	-1.60163300
N	2.90411800	0.32026600	-0.31011200
O	3.34605200	1.36354000	-0.72053300
O	3.52087300	-0.71812900	-0.09681800
N	-1.45696600	2.02100800	-0.14179300
O	-2.60540600	1.62544900	-0.18712900
O	-1.05318500	3.15669400	-0.24658700
N	0.96687300	-1.86382300	1.16853300
H	0.51430300	-2.77151000	1.09320500
H	1.97026400	-1.99293000	1.29096300
N	1.01747400	-1.65548700	-1.32199400
H	1.98546300	-1.97277200	-1.34401200
H	0.41318500	-2.46054600	-1.48916800

1,3-Diradical + N_2 (for the formation of compounds **P6-3 and P6-4**)

C	-0.73223000	-0.50374700	-0.11349000
C	0.74356000	-1.12821000	-0.10871400
C	1.52094300	0.17285300	-0.19853800
C	-0.48518900	0.95213600	-0.05515500
N	1.34975400	0.72970200	2.35869200
N	0.31417900	1.09782300	2.44468100
O	0.77502400	1.21921800	-0.27800500
N	-1.59725300	-1.08724500	0.99257800
O	-2.10726700	-0.31625300	1.76466800
O	-1.67812900	-2.29698800	0.99652300
N	-1.41155200	-0.80131400	-1.47655300
O	-1.29573000	0.08539800	-2.28634000
O	-1.91871900	-1.88174900	-1.62909900
N	2.91613800	0.29912700	-0.36552700
O	3.38289100	1.36858800	-0.68903200
O	3.53485700	-0.74543500	-0.14770200
N	-1.43981900	1.99273500	-0.18452700
O	-2.59849700	1.61095100	-0.21308700
O	-1.03031300	3.13435500	-0.24314700
N	0.99674000	-1.79689400	1.14299600

H	0.54694900	-2.70973400	1.15246900
H	2.00325400	-1.91205600	1.25227200
N	0.97465100	-1.81365200	-1.36133600
H	1.95678300	-2.08251100	-1.40746000
H	0.40259100	-2.65682900	-1.41852800

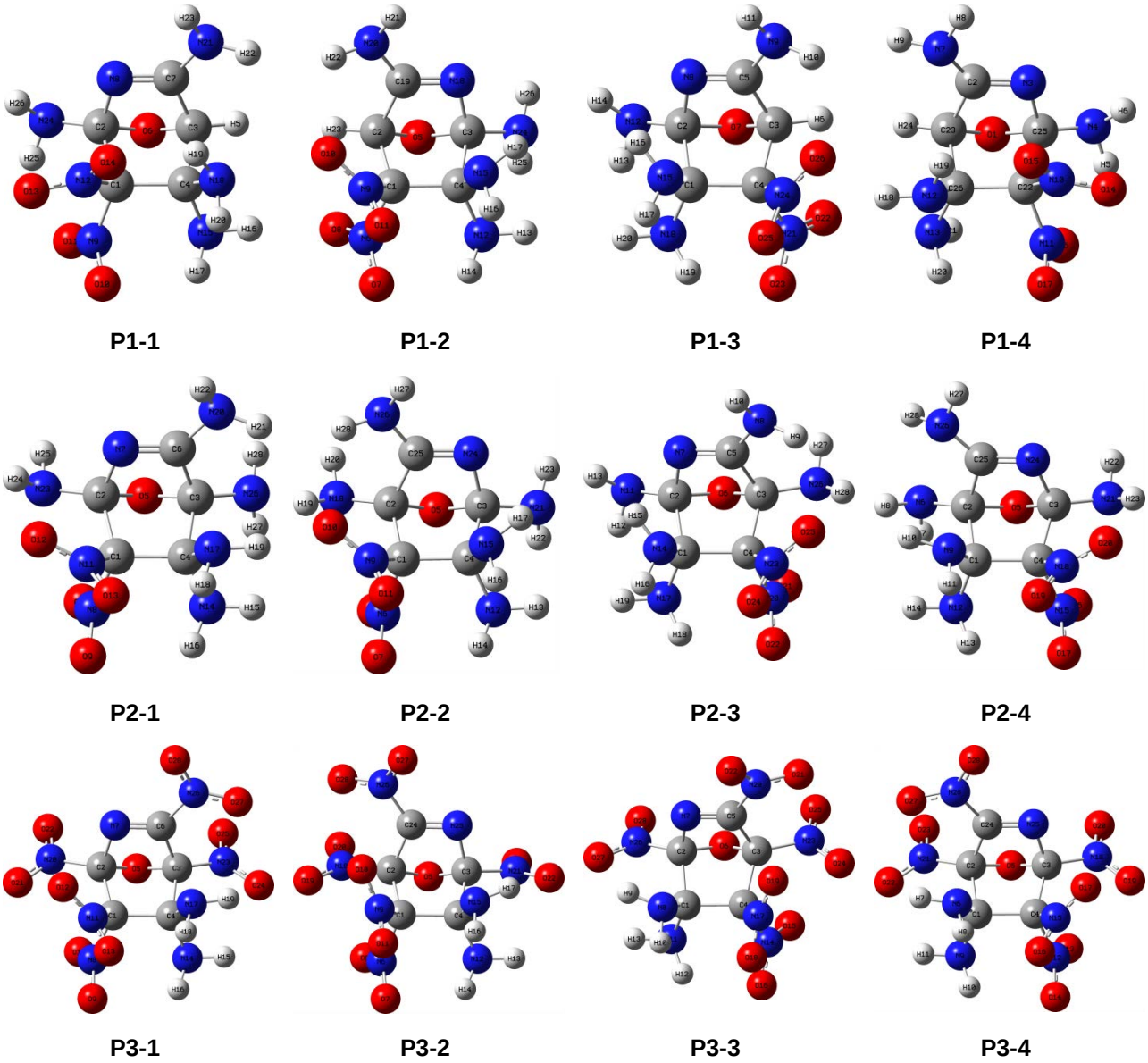


Fig. S3 The optimized structures of the compounds **P1-1~P3-4**

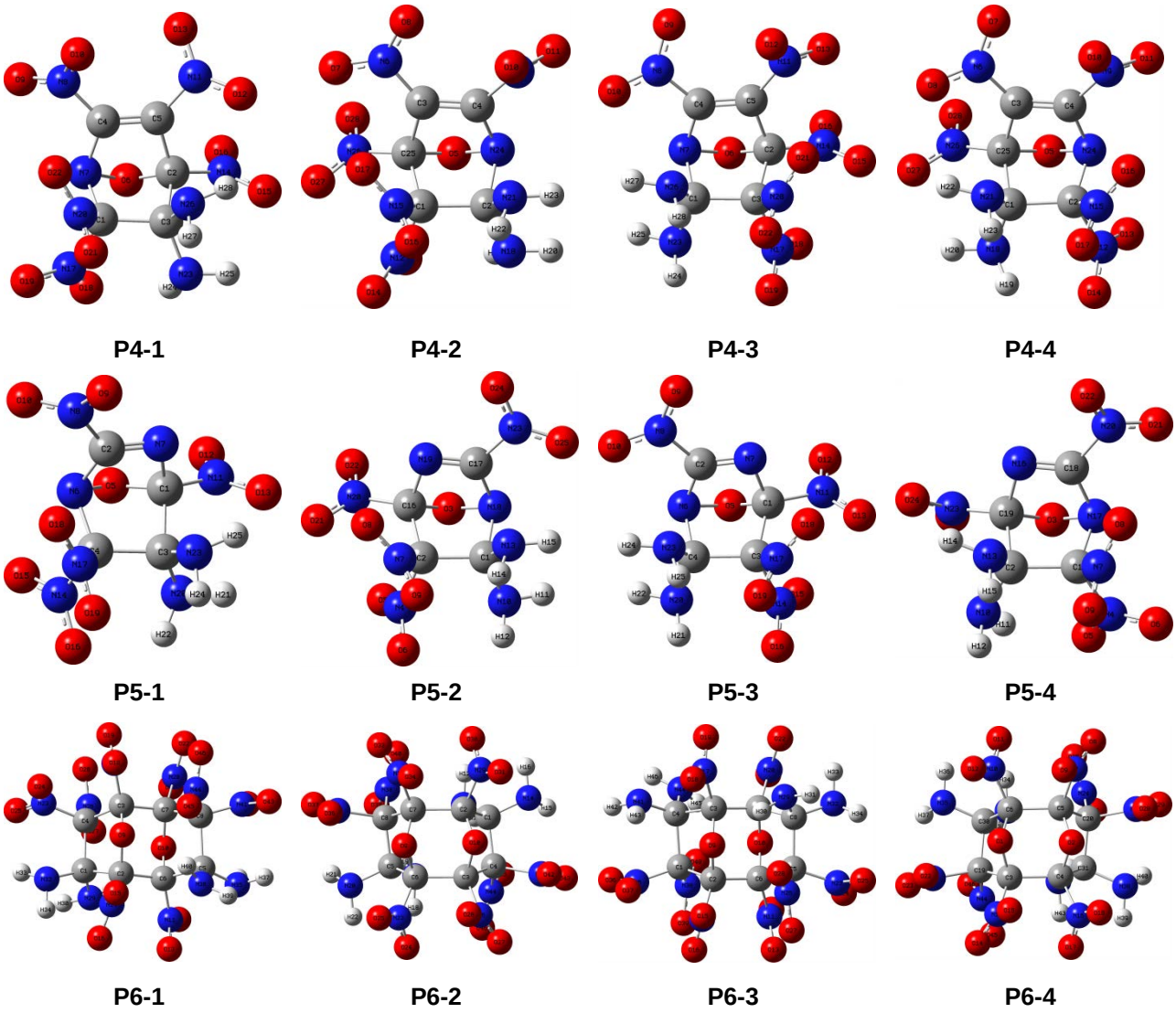


Fig. S4 The optimized structures of the compounds **P4-1~P6-4**

Table S3 Bond lengths (BL) and Laplacian bond order (LBO) of the compounds **P1-1~P1-4**

Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO
P1-1			**P1-2**		2b	**P1-3**			**P1-4**		
C1-C2	**1.6367**	**0.6203**	C1-C2	1.5480	0.9192	**C1-C2**	**1.6163**	**0.7535**	C2-C23	1.5195	1.0527
C1-C4	1.6044	0.7279	**C1-C4**	**1.5848**	**0.7935**	C1-C4	1.5925	0.7604	**C22-C25**	**1.6251**	**0.6664**
C3-C4	1.5709	0.8778	C2-C19	1.5370	0.9883	C3-C4	1.5458	0.9246	C22-C26	1.6173	0.6866
C3-C7	1.5238	1.0371	C3-C4	1.5934	0.8357	C3-C5	1.5371	0.9897	C23-C26	1.5786	0.8400
C1-N9(O2)	**1.5130**	**0.6190**	**C1-N6(O2)**	**1.5411**	**0.5260**	C1-N15(H2)	1.4431	0.8384	C2-N7(H2)	1.3557	1.1844
C1-N12(O2)	1.5050	0.6376	C1-N9(O2)	1.5136	0.6172	C1-N18(H2)	1.4487	0.8340	C25-N3	1.4607	0.7942
C2-N8	1.4611	0.7925	C3-N18	1.4603	0.7952	C2-N8	1.4635	0.7792	C25-N4(O2)	1.3982	1.0661
C2-N24(H2)	1.3956	1.0721	C3-N24(H2)	1.4085	1.0278	C2-N12(H2)	1.4040	1.0347	**C22-N10(O2)**	**1.5068**	**0.6364**
C4-N15(H2)	1.4460	0.8538	C4-N12(H2)	1.4508	0.8237	**C4-N21(O2)**	**1.5406**	**0.5235**	**C22-N11(O2)**	**1.5048**	**0.6353**
C4-N18(H2)	1.4476	0.8294	C4-N15(H2)	1.4479	0.8315	C4-N24(O2)	1.5124	0.6207	C26-N12(H2)	1.4289	0.9119
C7-N21(H2)	1.3507	1.2028	C19-N20(H2)	1.3549	1.2003	C5-N9(H2)	1.3541	1.2034	C26-N13(H2)	1.4435	0.8494
C2-O6	**1.4292**	**0.3597**	C2-O5	1.4173	0.3727	**C2-O7**	**1.4462**	**0.3151**	C23-O1	1.4247	0.3453
C3-O6	1.4160	0.3739	**C3-O5**	**1.4611**	**0.2711**	C3-O7	1.4168	0.3726	**C25-O1**	**1.4386**	**0.3331**
C7=N8	1.2923	1.5729	N18=C19	1.2895	1.6013	C5=N8	1.2903	1.5923	C2=N3	1.2907	1.5865

Table S4 Bond lengths (BL) and Laplacian bond order (LBO) of the compounds **P2-1~P2-4**

Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO
P2-1			**P2-2**			**P2-3**			**P2-4**		
C1-C2	1.5774	0.8468	C1-C2	1.5671	0.8628	C1-C2	1.6133	0.7646	**C1-C2**	**1.6082**	**0.7582**
C1-C4	**1.5814**	**0.8244**	**C1-C4**	**1.5915**	**0.7747**	**C1-C4**	**1.6007**	**0.7375**	C1-C4	1.5793	0.8262
C3-C4	1.5849	0.8437	C2-C25	1.5604	0.9120	C3-C4	1.5645	0.8709	C2-C25	1.5252	1.0457
C3-C6	1.5253	1.0460	C3-C4	1.5912	0.8431	C3-C5	1.5623	0.9062	C3-C4	1.5689	0.8765
C1-N8(O2)	**1.5495**	**0.5062**	**C1-N6(O2)**	**1.5510**	**0.5031**	C1-N14(H2)	1.4399	0.8470	C1-N9(H2)	1.4485	0.8264
C1-N11(O2)	1.5169	0.6148	C1-N9(O2)	1.5110	0.6264	C1-N17(H2)	1.4495	0.8343	C1-N12(H2)	1.4564	0.8010
C2-N7	1.4827	0.7048	C2-N18(H2)	1.4211	0.9498	C2-N7	1.4672	0.7635	C2-N6(H2)	1.4284	0.9223
C2-N23(H2)	1.4182	0.9979	C3-N21(H2)	1.4112	1.0147	C2-N11(H2)	1.4083	1.0210	C3-N21(H2)	1.4148	1.0109
C3-N26(H2)	1.4132	0.9687	C3-N24	1.4639	0.7783	C3-N26(H2)	1.4205	0.9527	C3-N24	1.4844	0.6997
C4-N14(H2)	1.4586	0.7966	C4-N12(H2)	1.4511	0.8252	**C4-N20(O2)**	**1.5486**	**0.5059**	**C4-N15(O2)**	**1.5540**	**0.4945**
C4-N17(H2)	1.4549	0.8109	C4-N15(H2)	1.4476	0.8330	C4-N23(O2)	1.5084	0.6320	C4-N18(O2)	1.5166	0.6152
C6-N20(H2)	1.3558	1.1883	C25-N26(H2)	1.3573	1.1819	C5-N8(H2)	1.3562	1.1857	C25-N26(H2)	1.3605	1.1704
C2-O5	1.4253	0.3689	C2-O5	1.4223	0.3692	**C2-O6**	**1.4345**	**0.3423**	C2-O5	1.4168	0.3838
C3-O5	**1.4409**	**0.3035**	**C3-O5**	**1.4504**	**0.2936**	C3-O6	1.4204	0.3784	**C3-O5**	**1.4381**	**0.3349**
C6=N7	1.2882	1.6093	N24=C25	1.2868	1.6148	C5=N7	1.2878	1.6047	N24=C25	1.2870	1.6184

Table S5 Bond lengths (BL) and Laplacian bond order (LBO) of the compounds **P3-1~P3-4**

Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO
P3-1			**P3-2**			**P3-3**			**P3-4**		
C1-C2	1.5612	0.8905	C1-C2	1.5606	0.8793	C1-C2	1.5851	0.8233	C1-C2	1.5822	0.8266
C1-C4	**1.6018**	**0.7492**	**C1-C4**	**1.6027**	**0.7368**	**C1-C4**	**1.6029**	**0.7363**	**C1-C4**	**1.6018**	**0.7491**
C3-C4	1.5822	0.8267	C2-C24	1.5402	0.9245	C3-C4	1.5607	0.8791	C2-C24	1.5335	0.9492
C3-C6	1.5335	0.9492	C3-C4	1.5852	0.8230	C3-C5	1.5403	0.9243	C3-C4	1.5612	0.8907
C1-N8(O2)	**1.5509**	**0.5135**	**C1-N6(O2)**	**1.5388**	**0.5488**	C1-N8(H2)	1.4419	0.8592	C1-N6(H2)	1.4518	0.8237
C1-N11(O2)	1.5180	0.6225	C1-N9(O2)	1.5228	0.6036	C1-N11(H2)	1.4433	0.8516	C1-N9(H2)	1.4366	0.8735
C2-N7	1.4767	0.7269	C2-N18(O2)	1.5065	0.6854	C2-N7	1.4710	0.7453	C2-N21(O2)	1.4997	0.6979
C2-N20(O2)	1.5117	0.6864	C3-N21(O2)	1.4995	0.7179	C2-N26(O2)	1.4996	0.7177	C3-N18(O2)	1.5116	0.6867
C3-N23(O2)	1.4997	0.6979	C3-N25	1.4710	0.7454	C3-N23(O2)	1.5064	0.6857	C3-N25	1.4767	0.7267
C4-N14(H2)	1.4366	0.8736	C4-N12(H2)	1.4433	0.8516	**C4-N14(O2)**	**1.5386**	**0.5497**	**C4-N12(O2)**	**1.5508**	**0.5138**
C4-N17(H2)	1.4519	0.8235	C4-N15(H2)	1.4419	0.8592	C4-N17(O2)	1.5229	0.6035	C4-N15(O2)	1.5180	0.6222
C6-N26(O2)	1.4702	0.7986	C24-N26(O2)	1.4713	0.7973	C5-N20(O2)	1.4713	0.7976	C24-N26(O2)	1.4702	0.7987
C2-O5	1.4133	0.3960	**C2-O5**	**1.4160**	**0.3814**	C2-O6	1.4081	0.4113	**C2-O5**	**1.4107**	**0.3918**
C3-O5	**1.4107**	**0.3918**	C3-O5	1.4082	0.4112	**C3-O6**	**1.4160**	**0.3815**	C3-O5	1.4133	0.3960
C6=N7	1.2647	1.7885	C24=N25	1.2650	1.7837	C5=N7	1.2650	1.7836	C24=N25	1.2647	1.7886

Table S6 Bond lengths (BL) and Laplacian bond order (LBO) of the compounds **P4-1~P4-4**

Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO
P4-1			**P4-2**			**P4-3**			**P4-4**		
C1-C3	1.5956	0.7804	**C1-C2**	**1.6005**	**0.7686**	**C1-C3**	**1.6014**	**0.7557**	**C1-C2**	**1.5884**	**0.7966**
C2-C3	**1.5959**	**0.7591**	C1-C25	1.5650	0.8638	C2-C3	1.5584	0.8848	C1-C25	1.5785	0.8342
C2-C5	1.5249	0.9508	C3-C25	1.5275	0.9426	C2-C5	1.5319	0.9268	C3-C25	1.5278	0.9456
C1-N7	1.5036	0.6639	C1-N12(O2)	1.5438	0.5333	C1-N7	1.5265	0.5837	C1-N18(H2)	1.4405	0.8560
C1-N17(O2)	**1.5477**	**0.5473**	C1-N15(O2)	1.5142	0.6350	C1-N23(H2)	1.4323	0.9196	C1-N21(H2)	1.4472	0.8394
C1-N20(O2)	1.5109	0.6662	C2-N18(H2)	1.4167	0.9729	C1-N26(H2)	1.4395	0.8808	**C2-N12(O2)**	**1.5600**	**0.5011**
C2-N14(O2)	1.4996	0.6933	C2-N21(H2)	1.4317	0.9266	C2-N14(O2)	1.5120	0.6638	C2-N15(O2)	1.5163	0.6356
C3-N23(H2)	1.4276	0.9007	**C2-N24**	**1.5585**	**0.4613**	**C3-N17(O2)**	**1.5397**	**0.5446**	C2-N24	1.4888	0.7159
C3-N26(H2)	1.4392	0.8769	C3-N6(O2)	1.4411	0.8653	C3-N20(O2)	1.5189	0.6113	C3-N6(O2)	1.4379	0.8856
C4-N7	1.4531	0.8209	C4-N9(O2)	1.4635	0.8240	C4-N7	1.4485	0.8537	C4-N9(O2)	1.4612	0.8285
C4-N8(O2)	1.4591	0.8384	C4-N24	1.4373	0.8910	C4-N8(O2)	1.4491	0.8665	C4-N24	1.4491	0.8300
C5-N11(O2)	1.4407	0.8727	C25-N26(O2)	1.5086	0.6760	C5-N11(O2)	1.4527	0.8376	C25-N26(O2)	1.5030	0.6861
C2-O6	**1.4227**	**0.4077**	**C25-O5**	**1.4205**	**0.4168**	**C2-O6**	**1.4188**	**0.4264**	**C25-O5**	**1.4212**	**0.4154**
N7-O6	**1.4649**	**0.1522**	**N24-O5**	**1.4604**	**0.1594**	**N7-O6**	**1.4562**	**0.1690**	**N24-O5**	**1.4647**	**0.1532**
C4=C5	1.3347	1.8312	C3=C4	1.3353	1.8175	C4=C5	1.3324	1.8425	C3=C4	1.3335	1.8356

Table S7 Bond lengths (BL) and Laplacian bond order (LBO) of the compounds **P5-1~P5-4**

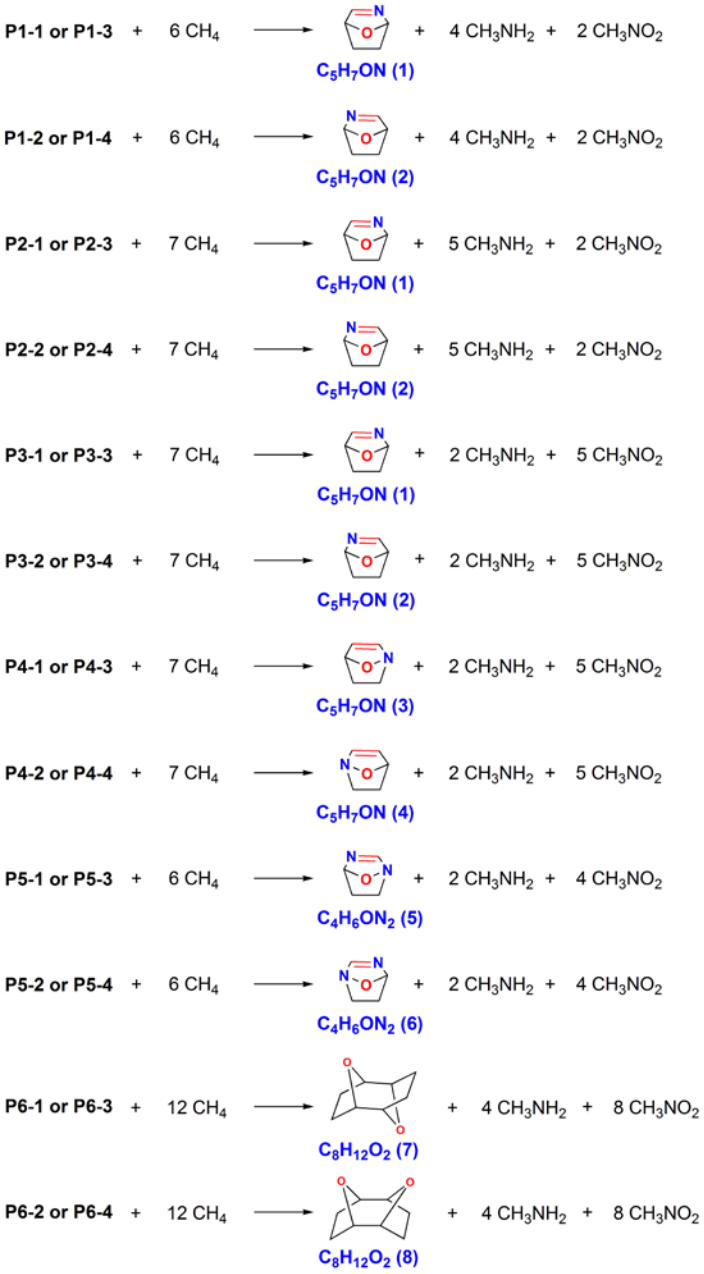
Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO
P5-1			**P5-2**			**P5-3**			**P5-4**		
C1-C3	1.5789	0.8359	**C1-C2**	**1.6011**	**0.7603**	C1-C3	1.5575	0.8964	**C1-C2**	**1.6197**	**0.6816**
C3-C4	**1.5877**	**0.7949**	C2-C16	1.5576	0.8961	**C3-C4**	**1.6011**	**0.7603**	C2-C19	1.5784	0.8352
C1-N7	1.4688	0.7468	C1-N10(H2)	1.4288	0.9306	C1-N7	1.4753	0.7233	**C1-N4(O2)**	**1.5401**	**0.5666**
C1-N11(O2)	1.4951	0.7313	C1-N13(H2)	1.4437	0.8655	C1-N11(O2)	1.5096	0.6935	C1-N7(O2)	1.5021	0.6861
C2-N6	1.4628	0.8048	C1-N18	1.5280	0.5814	C2-N6	1.4530	0.8626	C1-N17	1.5034	0.6582
C2-N8(O2)	1.4744	0.8044	**C2-N4(O2)**	**1.5427**	**0.5367**	C2-N8(O2)	1.4737	0.7987	C2-N10(H2)	1.4287	0.8919
C3-N20(H2)	1.4421	0.8503	C2-N7(O2)	1.5175	0.6188	**C3-N14(O2)**	**1.5428**	**0.5364**	C2-N13(H2)	1.4357	0.8897
C3-N23(H2)	1.4447	0.8480	C16-N19	1.4753	0.7236	C3-N17(O2)	1.5175	0.6188	C19-N16	1.4624	0.7690
C4-N6	1.4892	0.7122	C16-N20(O2)	1.5097	0.6931	C4-N6	1.5279	0.5815	C18-N17	1.4666	0.7960
C4-N14(O2)	**1.5516**	**0.5247**	C17-N18	1.4530	0.8627	C4-N20(H2)	1.4289	0.9304	C18-N20(O2)	1.4752	0.7974
C4-N17(O2)	1.5211	0.6184	C17-N23(O2)	1.4737	0.7988	C4-N23(H2)	1.4437	0.8657	C19-N23(O2)	1.4923	0.7377
C1-O5	**1.4152**	**0.4405**	**C16-O3**	**1.4148**	**0.4393**	**C1-O5**	**1.4149**	**0.4392**	**C19-O3**	**1.4226**	**0.4139**
N6-O5	**1.4664**	**0.1494**	**N18-O3**	**1.4548**	**0.1696**	**N6-O5**	**1.4548**	**0.1697**	**N17-O3**	**1.4679**	**0.1489**
C2=N7	1.2641	1.7979	C17=N19	1.2649	1.7979	C2=N7	1.2649	1.7981	N16=C18	1.2628	1.8103

Table S8 Bond lengths (BL) and Laplacian bond order (LBO) of the compounds **P6-1~P6-4**

Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO	Bonds	BL (Å)	LBO
P6-1			**P6-2**			**P6-3**			**P6-4**		
C1-C2	1.5884	0.8210	C1-C2	1.5978	0.7900	C1-C2	1.5605	0.8782	**C3-C4**	**1.6430**	**0.6312**
C1-C4	**1.6474**	**0.6033**	C1-C4	1.5962	0.7848	**C1-C4**	**1.7183**	**0.4037**	C3-C19	1.5534	0.9110
C2-C6	1.5575	0.9139	**C2-C7**	**1.6428**	**0.6316**	C2-C6	1.5791	0.8294	C4-C31	1.5978	0.7900
C3-C4	1.5695	0.8504	C3-C4	1.5534	0.9110	C3-C4	1.5792	0.8435	**C5-C6**	**1.6429**	**0.6314**
C3-C7	1.5791	0.8295	**C3-C6**	**1.6427**	**0.6320**	C3-C7	1.5575	0.9139	C5-C20	1.5534	0.9111
C5-C6	1.5792	0.8433	C5-C6	1.5977	0.7904	C5-C6	1.5695	0.8505	C6-C30	1.5978	0.7901
C5-C8	**1.7186**	**0.4031**	C5-C8	1.5962	0.7847	**C5-C8**	**1.6476**	**0.6028**	C19-C30	1.5962	0.7845
C7-C8	1.5605	0.8784	C7-C8	1.5532	0.9115	C7-C8	1.5885	0.8210	C20-C31	1.5962	0.7845
C1-N29(H2)	1.4211	0.9208	C1-N11(H2)	1.4349	0.8784	C1-N35(O2)	1.5034	0.6450	C3-N13(O2)	1.5488	0.5493
C1-N32(H2)	1.4432	0.8620	C1-N14(H2)	1.4561	0.8068	C1-N38(O2)	1.5437	0.5388	C4-N16(O2)	1.5167	0.6334
C2-N14(O2)	1.5310	0.6001	C2-N29(O2)	1.5169	0.6328	C2-N14(O2)	1.5470	0.5484	C5-N7(O2)	1.5488	0.5492
C3-N17(O2)	1.5500	0.5400	C3-N26(O2)	1.5488	0.5492	C3-N17(O2)	1.5231	0.6165	C6-N10(O2)	1.5167	0.6334
C4-N23(O2)	1.5297	0.5741	**C4-N41(O2)**	**1.6163**	**0.3480**	C4-N41(H2)	1.4255	0.9102	**C19-N21(O2)**	**1.6162**	**0.3480**
C4-N26(O2)	**1.5517**	**0.5219**	C4-N44(O2)	1.5126	0.6511	C4-N44(H2)	1.3997	1.0123	C19-N44(O2)	1.5124	0.6516
C5-N35(H2)	1.4255	0.9103	C5-N17(H2)	1.4351	0.8776	C5-N23(O2)	1.5298	0.5738	C20-N24(O2)	1.5125	0.6514
C5-N38(H2)	1.3996	1.0127	C5-N20(H2)	1.4560	0.8070	**C5-N26(O2)**	**1.5516**	**0.5223**	**C20-N27(O2)**	**1.6163**	**0.3480**
C6-N11(O2)	1.5230	0.6166	C6-N23(O2)	1.5170	0.6324	C6-N11(O2)	1.5499	0.5401	C30-N32(H2)	1.4349	0.8784
C7-N20(O2)	1.5471	0.5483	C7-N32(O2)	1.5488	0.5493	C7-N20(O2)	1.5311	0.6001	C30-N35(H2)	1.4562	0.8065
C8-N41(O2)	1.5033	0.6453	**C8-N35(O2)**	**1.6166**	**0.3473**	C8-N29(H2)	1.4210	0.9211	C31-N38(H2)	1.4562	0.8065
C8-N44(O2)	1.5436	0.5391	C8-N38(O2)	1.5124	0.6515	C8-N32(H2)	1.4432	0.8620	C31-N41(H2)	1.4349	0.8784

Continued to **Table S8**

Bonds	BL/Å	LBO	Bonds	BL/Å	LBO	Bonds	BL/Å	LBO	Bonds	BL/Å	LBO
P6-1			**P6-2**			**P6-3**			**P6-4**		
C2-O9	1.4134	0.3597	C2-O10	1.3915	0.4407	C2-O9	1.4166	0.3624	**C3-O1**	**1.4106**	**0.3892**
C3-O9	1.4046	0.3992	**C3-O10**	**1.4107**	**0.3892**	**C3-O9**	**1.4206**	**0.3384**	C6-O1	1.3915	0.4407
C6-O10	**1.4206**	**0.3383**	C6-O9	1.3915	0.4406	C6-O10	1.4046	0.3993	C4-O2	1.3915	0.4407
C7-O10	1.4166	0.3623	**C7-O9**	**1.4107**	**0.3891**	C7-O10	1.4134	0.3596	**C5-O2**	**1.4106**	**0.3893**



Scheme S1 Isodesmic reactions for the designed bridge-ring energetic compounds

Table S9 E_0, ZPE, H_T and $\Delta H_{f,\,gas}$ of the reference compounds

Compd.	E_0 [a] (au)	ZPE [b] (au)	H_T [b] (au)	$\Delta H_{f,\,gas}$ (kJ·mol^{-1})
CH_4	-40.5441	0.0444	0.0038	-74.60 [c]
CH_3-NH_2	-95.9157	0.0632	0.0043	-22.50 [c]
CH_3-NO_2	-245.1422	0.0492	0.0053	-80.80 [c]
C_5H_7ON (1)	-324.8428	0.1159	0.0058	-18.43 [d]
C_5H_7ON (2)	-324.8428	0.1159	0.0058	-18.43 [d]
C_5H_7ON (3)	-324.7753	0.1144	0.0059	161.30 [d]
C_5H_7ON (4)	-324.7753	0.1144	0.0059	161.29 [d]
$C_4H_6ON_2$ (5)	-340.8354	0.1035	0.0057	159.78 [d]
$C_4H_6ON_2$ (6)	-340.8354	0.1035	0.0057	159.78 [d]
$C_8H_{12}O_2$ (7)	-462.7472	0.1918	0.0079	-329.47 [d]
$C_8H_{12}O_2$ (8)	-462.7272	0.1921	0.0079	-271.75 [d]

[a] Calculated at b3lyp/def2QZVPP level. [b] Calculated at b3lyp/6-31g(d) level. [c] Obtained from http://webbook.nist.gov. [d] Calculated at G2 level.

Table S10 $\Delta H_{f,\,gas}$, ΔH_{sub} and $\Delta H_{f,\,solid}$ of the designed compounds and the related calculation parameters

Compd.	E_0 [a] (au)	ZPE [b] (au)	H_T [b] (au)	A [c] (Å^2)	$v\sigma_{tot}^2$ [c] (kcal·mol^{-1})^2	$\Delta H_{f,\,gas}$ (kJ·mol^{-1})	ΔH_{sub} (kJ·mol^{-1})	$\Delta H_{f,\,solid}$ (kJ·mol^{-1})
P1-1	-955.5984	0.1864	0.0160	213.994	51.968	-39.60	113.34	-152.94
P1-2	-955.6003	0.1868	0.0158	214.219	32.515	-44.09	103.04	-147.14
P1-3	-955.5942	0.1858	0.0162	213.994	51.968	-39.60	113.34	-152.94
P1-4	-955.6008	0.1867	0.0158	213.688	44.127	-45.66	109.28	-154.94
P2-1	-1010.9823	0.2027	0.0176	223.656	55.222	-23.75	119.60	-143.35
P2-2	-1010.9799	0.2023	0.0175	222.290	48.092	-18.62	115.49	-134.11
P2-3	-1010.9735	0.2013	0.0178	222.580	58.987	-3.84	120.78	-124.62
P2-4	-1010.9711	0.2017	0.0178	224.016	62.897	3.67	123.22	-119.55
P3-1	-1458.5427	0.1584	0.0211	257.586	15.659	109.08	113.85	-4.78
P3-2	-1458.5436	0.1581	0.0212	257.137	19.643	106.27	116.87	-10.60
P3-3	-1458.5436	0.1581	0.0212	257.136	19.675	106.30	116.90	-10.59
P3-4	-1458.5427	0.1584	0.0211	257.585	15.631	109.05	113.83	-4.77
P4-1	-1458.4766	0.1575	0.0214	260.618	18.462	287.34	117.95	169.39
P4-2	-1458.4818	0.1572	0.0214	258.923	23.328	272.98	120.65	152.33
P4-3	-1458.4789	0.1572	0.0214	256.128	21.876	280.46	117.99	162.47
P4-4	-1458.4757	0.1575	0.0214	260.262	17.968	289.70	117.35	172.35
P5-1	-1269.9426	0.1436	0.0186	238.093	21.199	283.62	107.53	176.09
P5-2	-1269.9458	0.1435	0.0185	234.940	22.306	274.80	106.68	168.12
P5-3	-1269.9458	0.1435	0.0185	234.936	22.259	274.78	106.64	168.13
P5-4	-1269.9441	0.0187	0.1434	238.565	22.204	279.82	108.52	171.30
P6-1	-2320.9418	0.2705	0.0335	336.477	20.823	-34.22	170.39	-204.61
P6-2	-2320.9081	0.2716	0.0327	336.329	19.543	59.83	169.30	-109.47
P6-3	-2320.9418	0.2705	0.0335	336.475	20.777	-34.22	170.36	-204.58
P6-4	-2320.9081	0.2716	0.0327	336.332	19.498	59.84	169.26	-109.43

[a] Calculated at b3lyp/def2QZVPP level. [b] Calculated at b3lyp/6-31g(d) level. [c] Calculated by Multiwfn program.

Table S11 Surface electrostatic potential parameters of the designed bridge-ring energetic molecules

Compd.	A_s	A_s^+	A_s^-	A_s^+/A_s	V_s	V_s^+	V_s^-	V_s^+/V_s^-
P1-1	213.99	97.26	116.74	45.45%	0.88	22.05	-16.75	-1.32
P1-2	214.22	98.01	116.21	45.75%	0.68	18.52	-14.35	-1.29
P1-3	214.54	98.04	116.50	45.70%	1.14	21.23	-15.77	-1.35
P1-4	213.69	95.64	118.05	44.76%	0.70	21.90	-16.48	-1.33
P2-1	223.66	101.02	122.64	45.17%	-0.12	22.48	-18.73	-1.20
P2-2	222.29	105.05	117.24	47.26%	0.22	19.61	-17.15	-1.14
P2-3	222.58	105.03	117.55	47.19%	0.56	22.26	-18.84	-1.18
P2-4	224.02	97.94	126.08	43.72%	-0.05	25.11	-19.59	-1.28
P3-1	257.59	113.51	144.08	44.07%	3.82	18.96	-8.11	-2.34
P3-2	257.14	106.97	150.16	41.60%	3.23	19.95	-8.68	-2.30
P3-3	257.14	106.89	150.25	41.57%	3.23	19.96	-8.68	-2.30
P3-4	257.58	113.64	143.95	44.12%	3.82	18.94	-8.12	-2.33
P4-1	260.62	125.75	134.87	48.25%	4.31	17.03	-7.54	-2.26
P4-2	258.92	108.68	150.24	41.98%	3.31	21.08	-9.54	-2.21
P4-3	256.13	107.47	148.66	41.96%	3.20	21.27	-9.87	-2.16
P4-4	260.26	119.02	141.24	45.73%	4.01	18.31	-8.03	-2.28
P5-1	238.09	103.93	134.16	43.65%	3.30	19.15	-8.99	-2.13
P5-2	234.94	96.75	138.19	41.18%	3.08	21.80	-10.03	-2.17
P5-3	234.94	96.88	138.05	41.24%	3.08	21.77	-10.04	-2.17
P5-4	238.56	104.75	133.82	43.91%	3.53	19.05	-8.62	-2.21
P6-1	336.48	126.59	209.89	37.62%	2.07	21.08	-9.40	-2.24
P6-2	336.33	123.90	212.43	36.84%	2.63	23.22	-9.37	-2.48
P6-3	336.48	126.69	209.78	37.65%	2.07	21.07	-9.40	-2.24
P6-4	336.33	124.02	212.31	36.87%	2.63	23.19	-9.37	-2.47
FOX-7	149.74	76.59	73.15	51.15%	1.95	24.80	-21.99	-1.13
RDX	199.80	100.90	98.90	50.50%	4.20	21.40	-13.36	-1.60
HMX	241.50	121.76	119.75	50.42%	5.77	23.38	-12.14	-1.93
CL-20	307.47	153.53	153.94	49.93%	6.60	21.58	-8.33	-2.59

A_s, A_s^+ and A_s^- are the overall surface area, positive surface area and negative surface area respectively, in $Å^2$; V_s, V_s^+ and V_s^- are the overall average value, positive average value and negative average value respectively, in $kcal \cdot mol^{-1}$.

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