Comprehensive End-to-End Design of Novel High Energy Density Materials: II. Computational Modeling and Predictions

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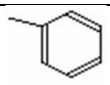
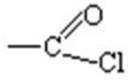
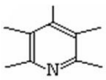
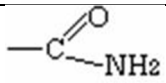
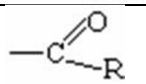
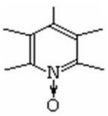
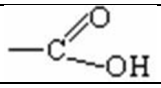
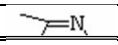
SUPPLEMENTARY INFORMATION

Table S1. Main structural components (functional groups of atoms) of the chemical formulas for calculations of physical and chemical parameters of EM with the Method of Atomic Contributions (MAC) method.

Group of atoms	Sum of components	Group of atoms	Sum of components
$-CH_3$	C_1+3H	– NO	N_6+O_9
$-CH_2-$	C_1+2H	> N-NO_2	$N_2+N_6+O_9$
$-CH=CH_2$	$2C_2+3H$	$-ONO_2$	$O_5+N_6+O_2+O_9$
>C=C<	$2C_2$	–S–	S
–C≡CH	$2C_3+H$	–SO	$S+O_2$
R–O–R	O_3	$-SO_2$	$S+2O_2$
–OH	O_1	–F	F
–O–OH	O_3+O_1+H	– Cl	Cl
R–O–O–R	$2O_3$		$6C_2+5H$
$-NH-NO_2$	$N_5+N_6+O_2+O_9+H$		
	C_2+O_9		$5C_2+N_8$
	$C_2+O_9+N_1+2H$		
	C_2+O_9		$5C_2+N_8+O_2$
	$C_2+H+O_1+O_9$		
–C≡N	C_3+N_7		$3C_2+H+N_2+N_8$

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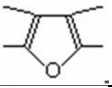
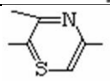
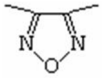
–C≡N→O	$C_3+N_7+O_2$		
$–NH_2$	$N_1 + 2H$		$4C_2+O_3$
$–NH·NH_2$	$2N_1+3_H$		
–N=N–	$2N_6$		$3C_2+N_8+S$
$–N_3$	$N_6+N_7+N_8$		
–C=N-OH	$C_2 + N_3 + O_1 + H$		$2C_2+2N_8+O_8$

Table S2 Atomic contributions used in calculations of formation enthalpy, ΔH^0_f, with MAC.

Atom type	**Contribution** in kcal/g*	**Atom type**	**Contribution** in kcal/g*	**Atom type**	**Contribution** in kcal/g*
C_1	-0.38	N_7	0.08	O_6	0.42
C_2	0.28	N_8	1.40	O_7	0.00
C_3	2.62	N_9	2.90	O_8	0.04
H	-1.21	N_{10}	-0.69	O_9	-3.24
N_1	0.15	N_{11}	0.82	O_{10}	-2.71
N_2	1.32	O_1	-2.70	F	-2.16
N_3	1.97	O_2	0.24	Cl	-0.15
N_4	-1.39	O_3	-1.57	S	0.71
N_5	5.31	O_4	-1.68		
N_6	3.45	O_5	-1.10		

*The selected units of the contribution (kcal/g) correspond to one gram of atomic mass of each type and therefore it serves as a vivid measure to compare relative contributions in energy in a simple way.

Table S3. Atomic contributions for determination of densities of molecular crystals with MAC.

Atom type	**Contribution (or correction)** in g/см^3	**Atom type**	**Contribution (or correction)** in g/см^3	**Atom type**	**Contribution (or correction) in** g/см^3
C_1	9.17	N_6	1.46	O_6	1.33
C_2	2.14	N_7	1.32	O_7	1.17
C_3	1.16	N_8	1.93	O_8	1.37
H	0.15	Correction N_9	-1.92	O_9	1.87
N_1	7.00	O_1	4.72	F	1.83
N_2	5.06	O_2	2.97	Cl	1.96
N_3	2.00	O_3	2.20	S	2.05
Correction N_4	-5.67	O_4	1.90		
Correction N_5	-29.79	O_5	2.13		

Modeling Thermal Decomposition in PHEs energetic molecules

Schematics of the most plausible decomposition mechanisms of PHE-1, PHE-2 and PHE-3 series compounds are depicted in Figures S1-S3. The calculated decomposition barriers, reaction energies and pre-exponential factors are collected in Table S4. The reactions rates plots of the corresponding mechanisms are shown in Figures S4. For PHEs molecules, we studied six most possible channels: (Figures S1-S3): ***1***) the homolytic cleavage of C-NO_2 bond, ***2***) the nitro-nitrite isomerization, ***3***) the central ring cleavage, ***4***) the concerted opening of the central 1,2,4-oxadiazole ring which takes place only in PHE-2 and PHE3, ***5***) the CN_2O_2 elimination via breaking of the outer nitro substituted oxadiazole ring, and ***6***) the CN_2O_3 elimination via breaking of the outer nitro substituted oxadiazole ring.

The homolytic C-NO_2 bond cleavage (mechanism 1) in PHEs compounds requires ~65 kcal/mol (Table S4). The CONO isomerization (mechanism 2), proceeding via a pseudo rotation of a nitro group accompanied by the C-NO_2 bond rupture and the formation of the C-ONO bond, requires ~47-50 kcal/mol. The lowest activation barrier (47.3 kcal/mol) was predicted for the PHE-2 molecule. Being an exothermic reaction, the CONO isomerization proceeds with the heat release of ~10-15 kcal/mol (Tables S4).

The cleavage of the central 1,2,4-oxadiazole ring (mechanism 3) in PHE-2 (66.6 kcal/mol) and PHE-3 (67.1 kcal/mol) molecules requires close energies as compared to LLM-191 (61.5 kcal/mol), LLM-192 (68.9 kcal/mol), LLM-200 (65.5 kcal/mol) and noticeably higher energies (by ~15-20 kcal/mol) than th cleavage of the central 1,2,5-oxadiazole ring in LLM-172 (48.4 kcal/mol) and LLM-175 (47.5 kcal/mol). The cleavage of the central 1,3,4-oxadiazole ring in the PHE-1 molecule has the highest activations barrier of 73.7 kcal/mol. An alternative to the central ring cleavage reaction, opening of central 1,2,4-oxadiazole ring in PHE-2 and PHE-3, requires ~62 kcal/mol.

Elimination of CN_2O_2 from the outer 1,3,4-oxadiazole ring in PHE-1 (81.7 kcal/mol) and 1,2,4-oxadiazole rings in PHE-2 (71.9 kcal/mol), PHE-3 (81.6 kcal/mol) requires significantly higher energies than elimination of CN_2O_2 from the outer 1,2,5-oxadiazole ring in LLM series compounds, ~ 48 kcal/mol. The calculated activation barrier for the CN_2O_3 moiety loss from the outer 1,3,4-oxadiazole rings of PHE-1 (58.4 kcal/mol) and PHE-3 (58.1 kcal/mol) molecules is ~8 kcal/mol higher than the energy of the CN_2O_3 elimination from the outer 1,3,4-oxadiazole ring of PHE-2 (50.1 kcal/mol) and 1,2,5-oxadiazole ring of LLM series compounds.

An analysis of the activation enthalpies, pre-exponential factors collected in Tables S4 and reaction rates depicted in Figures S4 confirm that decomposition of the PHE-1 and PHE-3 molecules occurred as a complex process, involving a competition of several mechanisms at different

temperatures. Thus, the CONO rearrangement is the dominating reaction at low temperatures. The homolytic C-NO_2 bond cleavage and the elimination of the CN_2O_3 fragment via a stepwise cleavage of the outer 1,3,4-oxadiazole ring are dominating reactions at high temperatures. The elimination of CN_2O_3 through breaking of an outer 1,2,4-oxadiazole ring in PHE-2 requires a lower energy than the similar process, involving 1,3,4-oxadiazole rings in PHE-1 and PHE-3 (Table S4). As a result, this process becomes the fastest reaction pathway in the decomposition of PHE-2 (Figure S4). The CONO rearrangement in PHE-2 proceeds at a slightly lower rate due to a low A-factor (Table S4, Figure S4). However, both reactions are likely to be triggered almost simultaneously during heating. The cleavage of the C-NO_2 bond in PHE-2 dominates in the overall decomposition only at high temperatures.

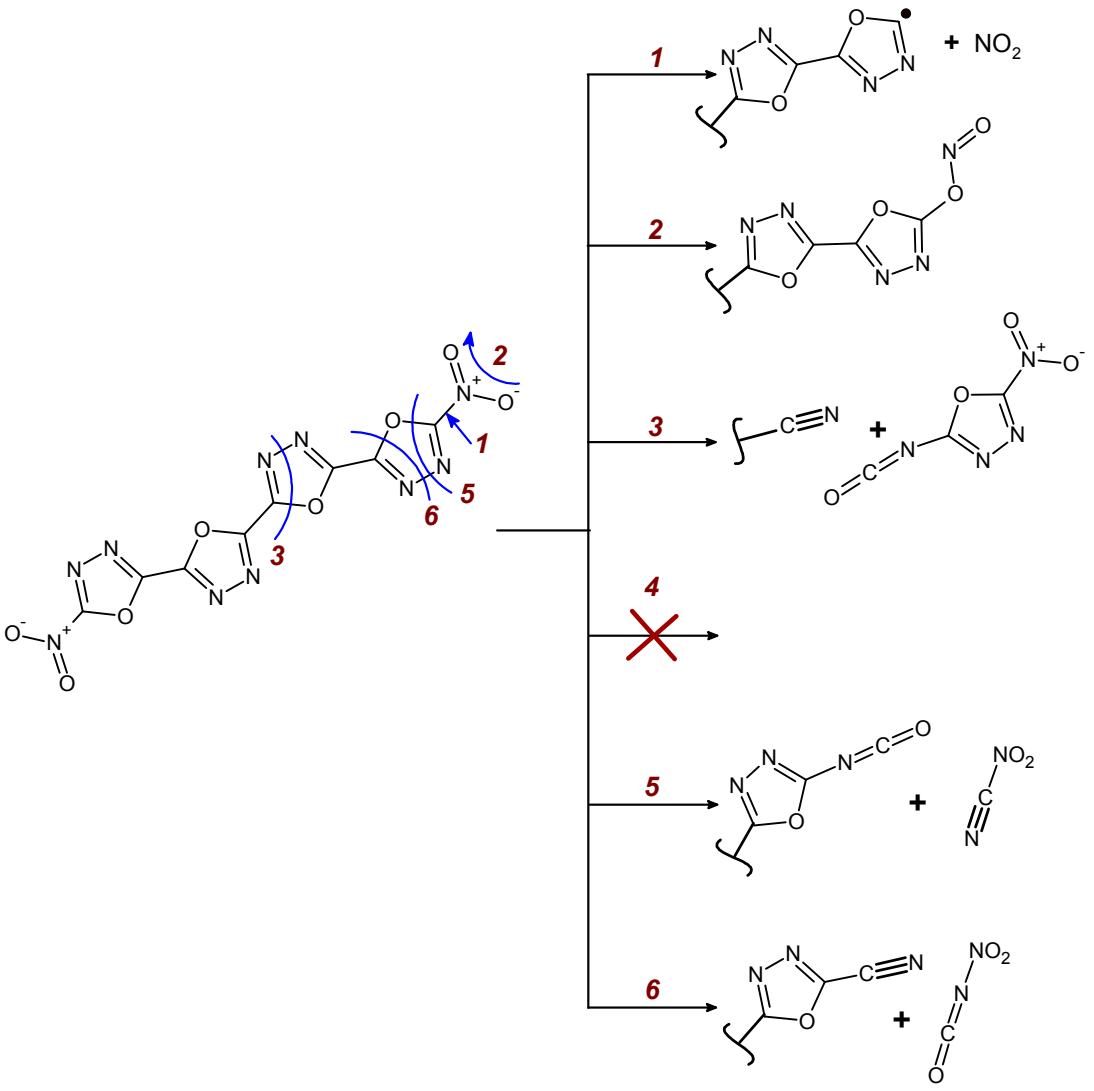


Figure S1 The sketched decomposition mechanisms of the most plausible initiation reactions in PHE-1 molecule.

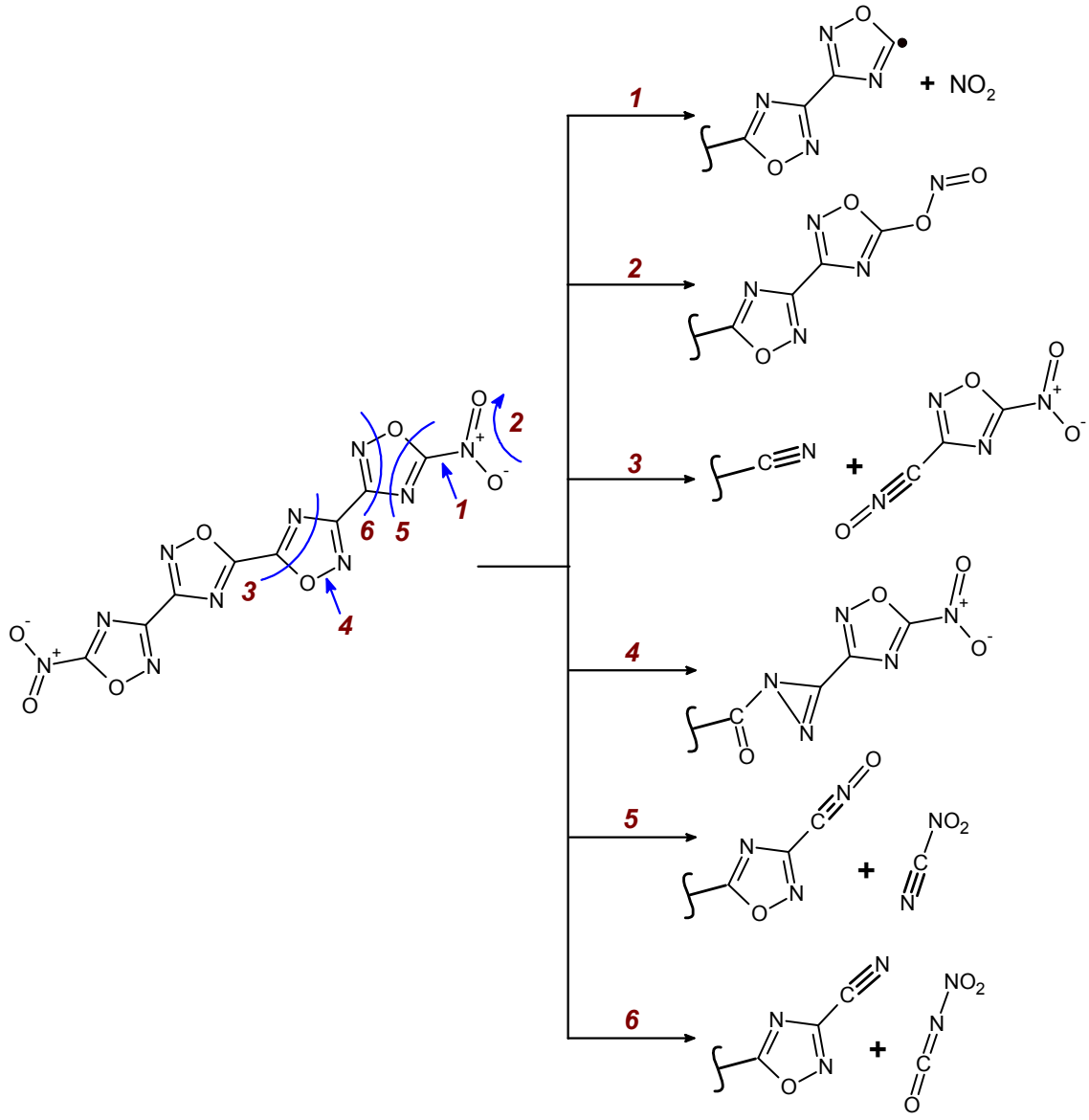


Figure S2 The sketched decomposition mechanisms of the most plausible initiation reactions in PHE-2 molecule.

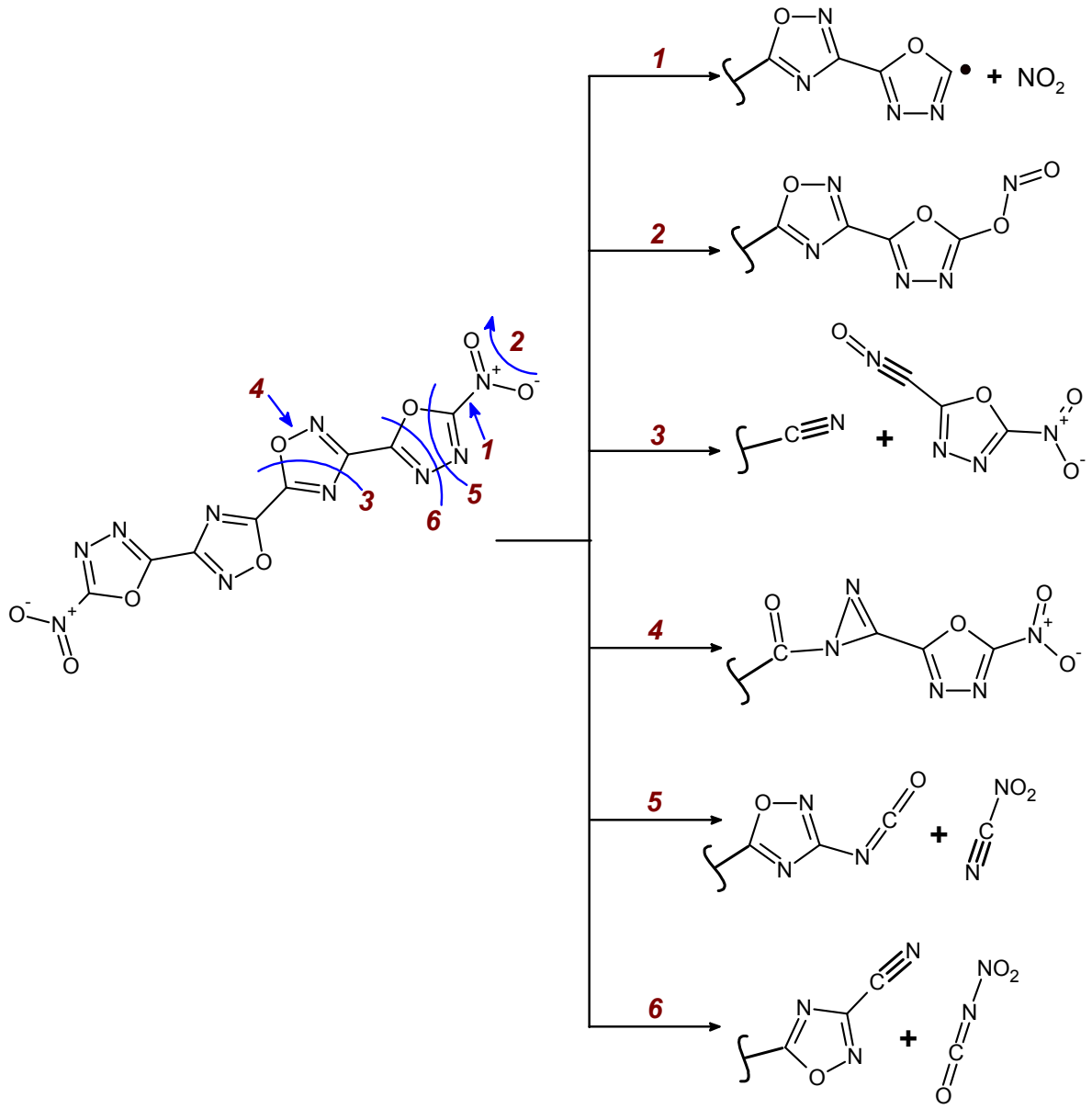


Figure S3 The sketched decomposition mechanisms of the most plausible initiation reactions in PHE-3 molecule.

Table S4. Activation enthalpies ($\Delta H^{\neq}_{298}$, kcal/mol), and pre-exponential factors (log(A, s^{-1})), and reaction enthalpies (given in parentheses in kcal/mol) of decomposition reactions in LLM-200, PHE-1, PHE-2, PHE-3 and TKX-55 compounds were calculated using M06/6-31+G(2df,p).

Decomposition mechanism		LLM-200		PHE-1		PHE-2		PHE-3		TKX-55	
		$\Delta H^{\neq}_{298}$	log(*A*)	$\Delta H^{\neq}_{298}$	log(*A*)	$\Delta H^{\neq}_{298}$	log(*A*)	$\Delta H^{\neq}_{298}$	log(*A*)	$\Delta H^{\neq}_{298}$	log(*A*)
NO_2 loss		64.1	17.4	66.3	17.7	64.2	17.6	66.6	17.7	64.0	17.9
CONO		52.9 (-10.3)	13.0	50.2 (-14.7)	13.3	47.3 (-14.4)	13.2	50.7 (-14.0)	13.4	55.7	13.6
CR cleavage		65.5 (50.4)	15.3	73.7 (-8.1)	15.7	66.6 (52.5)	15.3	67.1 (51.7)	15.5	69.2	15.0
CR opening		54.9 (51.4)	13.0	-	-	61.4 (44.0)	14.7	62.4 (44.6)	15.0	-	-
CN_2O_2 loss		48.8 (31.0)	15.0	81.7 (-1.4)	15.4	71.9 (58.5)	15.1	81.6 (-1.6)	15.6	-	-
CN_2O_3 loss	Step 1	50.7 (33.2)	14.6	35.5 (23.5)	15.2	49.7 (34.2)	15.0	36.1 (23.3)	15.4	-	-
	Step 2			58.4 (4.0)	16.1	50.1 (-3.6)	16.0	58.1 (3.7)	16.4	-	-

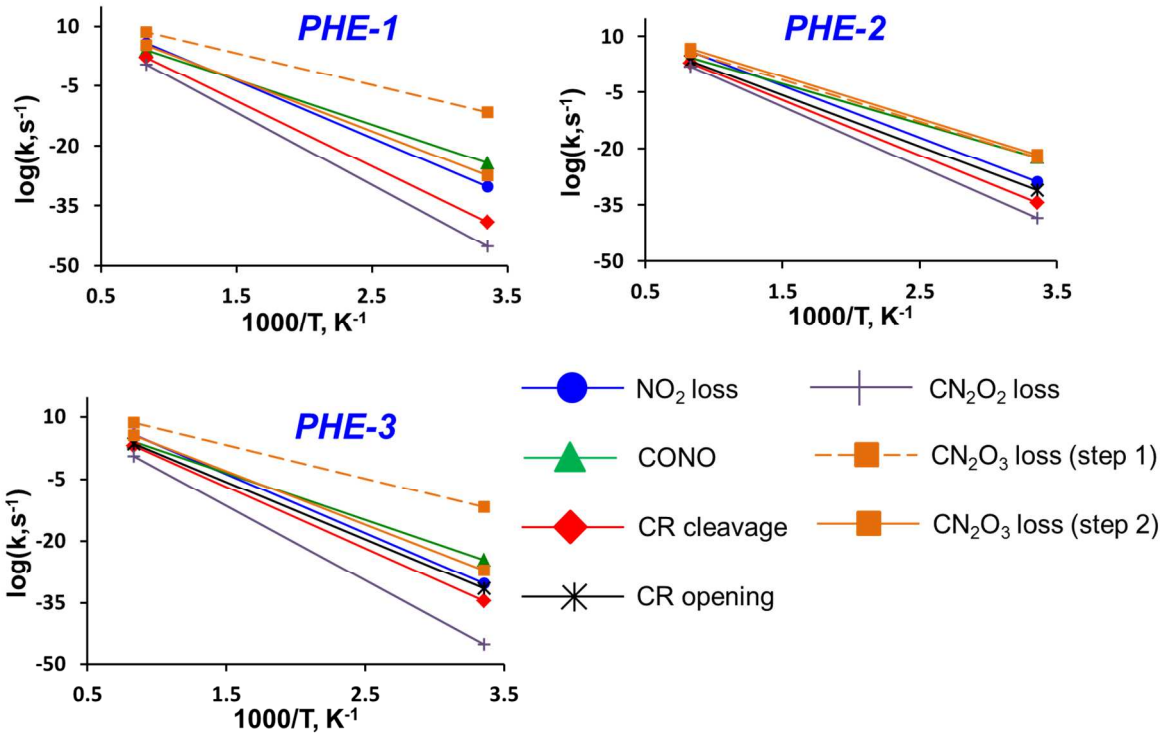


Figure S4 Reaction rates of the simulated decomposition channels of PHE-1, PHE-2 and PHE-3.

Modeling Thermal Decomposition of TKX-55

TKX-55[1] contains two central 1,3,4-oxadiazole rings and two outer 3-nitro-phenyl rings and demonstrates low thermal sensitivity. We simulated thermal decomposition of TKX-55 in order to reveal mechanisms that ensure high thermal stability of this compound. We studied three most plausible decomposition channels (Figure S5) on TKX-55 associated with ***1***) the homolytic loss of NO_2, ***2***) the CONO rearrangement and ***3***) the cleavage of the central 1,3,4-oxadiazole ring.

The calculated activation barriers and pre-exponential factors collected in Table S4 and reaction rates depicted in Figure S6 show that the NO_2 loss (mechanism 1), which requires 64 kcal/mol, dominates overall decomposition at a wide temperature range. The CONO isomerization (mechanism 2), with the activation barrier of 55.7 kca/mol, proceeds at lower rates due to low pre-exponential factor log(A, s^{-1}) ~13.6. The cleavage of the central 1,3,4-oxadiazole ring (mechanism 3) requires a high activation energy (69.2 kca/mol) and, thus, will proceed at low rates.

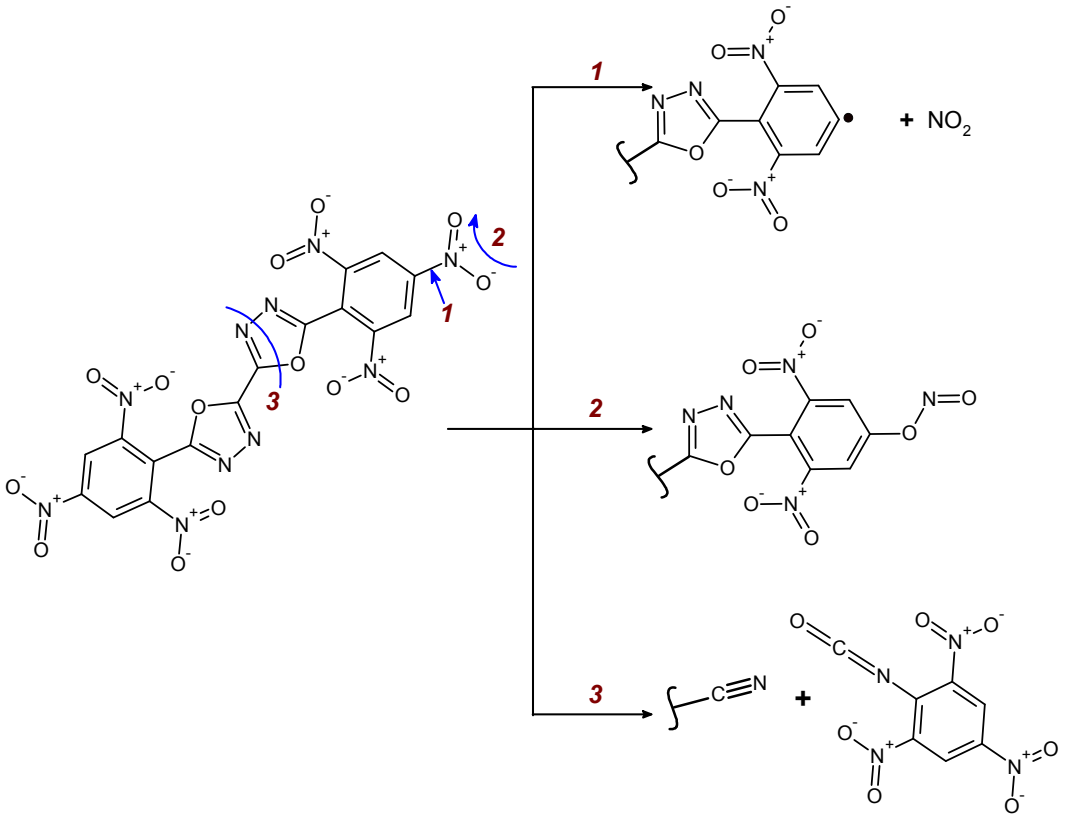


Figure S5. The sketched decomposition mechanisms of the most plausible initiation reactions in TKX-55 molecule.

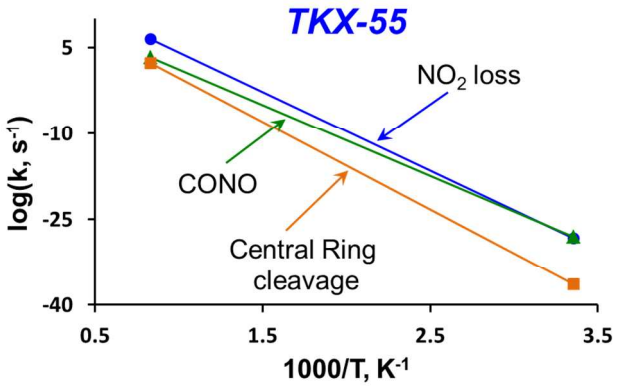


Figure S6. Reaction rates of the simulated decomposition channels of TKX-55.

Coordinates

Decomposition of PHE-1

Structure: Ground state equilibrium
Method: M06/6-31+G(2df,p)

7	0	5.747518	-0.192474	1.550381
6	0	6.710392	-0.224900	0.683675
6	0	6.686656	0.225050	-0.683626
8	0	7.848384	-0.751360	1.168595
8	0	5.548665	0.751510	-1.168546
7	0	7.649531	0.192624	-1.550332
6	0	7.489024	-1.042780	2.430358
6	0	5.908025	1.042930	-2.430309
7	0	6.261447	-0.731984	2.702318
7	0	7.135602	0.732134	-2.702269
6	0	8.464613	-1.642246	3.303905
8	0	8.106082	-1.933755	4.566188
6	0	9.242803	-2.454779	5.034520
7	0	9.695007	-1.954614	3.032679
7	0	10.208713	-2.494953	4.187330
7	0	9.263776	-2.909043	6.419389
8	0	8.233616	-2.771814	7.038493
8	0	10.308482	-3.374402	6.801527
6	0	4.932436	1.642396	-3.303856
8	0	5.290967	1.933905	-4.566139
6	0	4.154247	2.454929	-5.034471
7	0	3.702042	1.954764	-3.032630
7	0	3.188336	2.495103	-4.187281
7	0	4.133273	2.909193	-6.419339
8	0	5.163433	2.771964	-7.038444
8	0	3.088567	3.374552	-6.801478

Reaction: CONO isomerization
Structure: Transition State
Method: M06/6-31+G(2df,p)

7	0	5.725210	-0.436639	1.454217
6	0	6.746732	-0.297091	0.667979
6	0	6.768385	0.215348	-0.676423
8	0	7.905262	-0.694634	1.223511
8	0	5.609889	0.615574	-1.232587
7	0	7.789485	0.350699	-1.460429
6	0	7.493632	-1.095841	2.438431
6	0	6.021676	1.014775	-2.448742
7	0	6.218745	-0.963391	2.621299
7	0	7.299735	0.876922	-2.629923
6	0	8.471294	-1.606983	3.363854
8	0	8.059022	-2.010252	4.578427
6	0	9.216016	-2.401251	5.118122
7	0	9.750338	-1.739919	3.184411
7	0	10.241268	-2.268661	4.354400
7	0	9.190953	-2.922713	6.478611

8	0	8.106410	-2.960221	7.013388
8	0	10.256770	-3.262920	6.928978
6	0	5.051746	1.525053	-3.372523
8	0	5.492138	1.925599	-4.611119
6	0	4.348188	2.355849	-5.139720
7	0	3.783259	1.680353	-3.217515
7	0	3.293131	2.239140	-4.381302
7	0	4.305798	2.453000	-6.680530
8	0	3.842990	2.232206	-7.737372
8	0	4.455478	3.630335	-6.142032

Reaction: CONO isomerization
Structure: CONO isomer of PHE-1 (product)
Method: M06/6-31+G(2df,p)

7	0	-0.978752	-0.459308	1.448829
6	0	0.069348	-0.236361	0.718456
6	0	0.127220	0.324432	-0.605512
8	0	1.220661	-0.590862	1.317026
8	0	-1.022214	0.681231	-1.206015
7	0	1.176604	0.542033	-1.331104
6	0	0.775123	-1.057326	2.496070
6	0	-0.575152	1.145504	-2.386902
7	0	-0.512193	-1.000597	2.620532
7	0	0.715543	1.082813	-2.506251
6	0	1.734560	-1.548496	3.450759
8	0	1.287856	-2.016389	4.629661
6	0	2.437553	-2.364739	5.212429
7	0	3.026191	-1.607140	3.330520
7	0	3.489086	-2.150820	4.505093
7	0	2.376776	-2.935136	6.551638
8	0	1.271959	-3.048928	7.031534
8	0	3.437018	-3.234934	7.042410
6	0	-1.531640	1.634538	-3.341927
8	0	-1.081067	2.103887	-4.525411
6	0	-2.232498	2.487364	-5.116333
7	0	-2.816417	1.700845	-3.219481
7	0	-3.283757	2.272103	-4.378227
7	0	-3.375409	2.356168	-7.214669
8	0	-3.506920	2.982569	-8.137090
8	0	-2.168774	2.993804	-6.308251

Reaction: NO2 loss
Structure: C8N9O6 radical
Method: M06/6-31+G(2df,p)

7	0	5.749993	-0.197031	1.563864
6	0	6.711712	-0.228892	0.695316
6	0	6.687824	0.220998	-0.671921
8	0	7.850515	-0.755616	1.179233
8	0	5.549170	0.747632	-1.157215
7	0	7.650030	0.188628	-1.537635
6	0	7.492717	-1.047428	2.441456

6	0	5.907468	1.039697	-2.419672
7	0	6.265785	-0.736960	2.715156
7	0	7.135958	0.728555	-2.690854
6	0	8.469129	-1.647088	3.313804
8	0	8.111460	-1.938539	4.576601
6	0	9.248319	-2.459940	5.044301
7	0	9.699526	-1.960053	3.042104
7	0	10.213685	-2.500530	4.196564
7	0	9.270141	-2.914026	6.428864
8	0	8.240758	-2.776126	7.049501
8	0	10.314825	-3.380443	6.810819
6	0	4.932931	1.638726	-3.293422
8	0	5.300616	1.931729	-4.567700
6	0	4.162317	2.448819	-5.023945
7	0	3.706949	1.950931	-3.028372
7	0	3.184082	2.502162	-4.207438

Reaction: Central Ring Cleavage
Structure: Transition state
Meth**o**d: M06/6-31+G(2df,p)

7	0	8.123194	-2.639320	-0.175454
6	0	8.332336	-1.368045	-0.320414
6	0	8.462796	-0.657306	-1.537126
8	0	8.417481	-0.700986	0.844067
8	0	6.199983	0.537873	-1.186689
7	0	8.637200	-0.120690	-2.552208
6	0	8.229455	-1.691372	1.727351
6	0	6.474075	1.023381	-2.256486
7	0	8.053330	-2.852008	1.173903
7	0	7.319236	1.077444	-3.224709
6	0	8.248291	-1.374877	3.132893
8	0	8.021635	-2.359000	4.018932
6	0	8.124844	-1.687147	5.167969
7	0	8.467864	-0.221954	3.685761
7	0	8.384930	-0.434279	5.040699
7	0	7.936515	-2.428943	6.410322
8	0	7.695244	-3.607886	6.291524
8	0	8.042272	-1.784586	7.423370
6	0	5.600671	2.033834	-3.066618
8	0	4.557604	1.538795	-3.762603
6	0	3.925307	2.662397	-4.095011
7	0	5.605428	3.328427	-3.000670
7	0	4.484477	3.744995	-3.678056
7	0	2.697737	2.551978	-4.875029
8	0	2.333263	1.428125	-5.134950
8	0	2.174896	3.595064	-5.178532

Reaction: Central Ring Cleavage
Structure: C3N4O4 (product)
Meth**o**d: M06/6-31+G(2df,p)

8	0	-0.125844	-0.234342	-1.268559

6	0	-0.303902	0.762943	-1.821455
7	0	-0.383718	1.847152	-2.353473
6	0	-1.218124	2.520004	-3.160417
8	0	-2.357678	1.927970	-3.587174
6	0	-2.880108	2.906369	-4.341325
7	0	-1.070087	3.729304	-3.610993
7	0	-2.175330	3.976308	-4.391843
7	0	-4.149695	2.651378	-4.997940
8	0	-4.637196	1.557709	-4.808627
8	0	-4.592093	3.553309	-5.666113

Reaction: Central Ring Cleavage
Structure: C5N6O4 (product)
Method: M06/6-31+G(2df,p)

7	0	1.791372	-2.874755	-0.186708
6	0	2.083016	-1.626864	-0.380777
6	0	2.374232	-0.982335	-1.609154
8	0	2.096551	-0.901333	0.756234
7	0	2.611359	-0.458103	-2.610919
6	0	1.782716	-1.833016	1.669864
7	0	1.593827	-3.009937	1.163030
6	0	1.694419	-1.438837	3.052922
8	0	1.379548	-2.368917	3.970254
6	0	1.398201	-1.635091	5.085777
7	0	1.885008	-0.259051	3.558910
7	0	1.686868	-0.394469	4.912313
7	0	1.096640	-2.303653	6.346061
8	0	0.846736	-3.484940	6.273379
8	0	1.128590	-1.605553	7.328723

Reaction: CN2O2 loss
Structure: Transition state
Method: M06/6-31+G(2df,p)

7	0	5.806516	-0.497051	1.138424
6	0	6.903422	-0.140404	0.547198
6	0	7.047308	0.552205	-0.706385
8	0	8.011828	-0.481090	1.227351
8	0	5.943381	0.877433	-1.393928
7	0	8.147666	0.921887	-1.289948
6	0	7.485906	-1.086945	2.304991
6	0	6.472632	1.482209	-2.475107
7	0	6.190884	-1.121382	2.297524
7	0	7.765508	1.544602	-2.448584
6	0	8.378800	-1.608816	3.307322
8	0	7.852525	-2.213058	4.386646
6	0	8.961444	-2.545128	5.052091
7	0	9.676443	-1.576872	3.316189
7	0	10.059598	-2.201197	4.479227
7	0	8.809791	-3.243215	6.322928
8	0	7.673714	-3.464215	6.674797
8	0	9.835596	-3.526747	6.889719

6	0	5.524098	1.827029	-3.641298
8	0	5.093317	1.075095	-4.491334
6	0	3.957158	2.933469	-5.325602
7	0	5.488872	3.036829	-3.213800
7	0	4.294965	3.737449	-4.554248
7	0	3.399182	2.146322	-6.390770
8	0	4.054077	2.112926	-7.399596
8	0	2.342186	1.626900	-6.143435

Reaction: CN2O2 loss
Structure: C7N8O6 (product)
Method: M06/6-31+G(2df,p)

7	0	-0.631132	-0.847252	0.981878
6	0	0.443939	-0.222811	0.611002
6	0	0.637408	0.581935	-0.564658
8	0	1.471308	-0.379618	1.463816
8	0	-0.398984	0.734547	-1.416756
7	0	1.702987	1.207116	-0.941307
6	0	0.920039	-1.167729	2.403775
6	0	0.150533	1.527542	-2.364902
7	0	-0.315392	-1.469703	2.164163
7	0	1.387702	1.830714	-2.125121
6	0	1.727484	-1.572142	3.524948
8	0	1.174990	-2.359069	4.465037
6	0	2.203363	-2.506662	5.303783
7	0	2.967184	-1.272395	3.769014
7	0	3.278903	-1.896540	4.953493
7	0	1.999216	-3.321856	6.493786
8	0	0.897358	-3.804247	6.625128
8	0	2.952311	-3.430468	7.224889
6	0	-1.715345	1.767045	-3.842304
8	0	-2.755186	1.697483	-4.340225
7	0	-0.592521	1.911767	-3.416248

Reaction: CN2O3 loss (step 1)
Structure: Transition state
Method: M06/6-31+G(2df,p)

7	0	4.008467	0.071438	1.813299
6	0	5.223271	0.378225	1.483664
6	0	5.667605	1.090441	0.313921
8	0	6.140614	-0.035369	2.374616
8	0	4.760616	1.484064	-0.584773
7	0	6.887373	1.416073	-0.003440
6	0	5.364899	-0.633604	3.293957
6	0	5.540429	2.082794	-1.512930
7	0	4.101574	-0.596391	3.006925
7	0	6.804874	2.054802	-1.203945
6	0	5.993897	-1.224279	4.447325
8	0	5.219477	-1.823380	5.367830
6	0	6.141927	-2.227527	6.244492
7	0	7.258886	-1.260218	4.734942

7	0	7.352705	-1.928994	5.931952
7	0	5.686654	-2.944336	7.430272
8	0	4.492340	-3.111029	7.522678
8	0	6.551865	-3.294476	8.193212
6	0	4.945888	2.639266	-2.657938
8	0	4.045341	1.150948	-3.864516
6	0	3.792836	1.990427	-4.711713
7	0	4.685053	3.445766	-3.503433
7	0	4.086338	3.308778	-4.673351
7	0	3.055459	1.597002	-5.956876
8	0	3.700174	1.609610	-6.974600
8	0	1.899234	1.293196	-5.802344

Reaction: CN2O3 loss (step 1)
Structure: Product
Method: M06/6-31+G(2df,p)

7	0	-0.070823	-1.376520	0.641548
6	0	0.406870	-0.178718	0.768827
6	0	0.231530	0.940180	-0.118885
8	0	1.147667	-0.012649	1.877699
8	0	-0.509259	0.770531	-1.228619
7	0	0.706406	2.140341	0.003220
6	0	1.079397	-1.237552	2.427126
6	0	-0.442446	1.998384	-1.782621
7	0	0.372935	-2.074759	1.735596
7	0	0.266019	2.839203	-1.087321
6	0	1.769385	-1.473956	3.669111
8	0	1.704006	-2.697783	4.220665
6	0	2.443761	-2.516652	5.317469
7	0	2.477021	-0.633821	4.360455
7	0	2.923812	-1.332273	5.456592
7	0	2.621988	-3.652616	6.214421
8	0	2.074625	-4.679532	5.884697
8	0	3.297739	-3.445901	7.191183
6	0	-1.105671	2.242627	-2.992186
8	0	-3.135433	0.754076	-5.346643
6	0	-2.910690	1.873931	-5.663137
7	0	-1.636103	2.490306	-3.990299
7	0	-2.169143	2.860317	-5.067718
7	0	-3.520458	2.442585	-6.988099
8	0	-4.209585	1.664387	-7.593949
8	0	-3.253920	3.581865	-7.281896

Reaction: CN2O3 loss (step 2)
Structure: Transition state
Method: M06/6-31+G(2df,p)

7	0	5.700839	-0.376684	1.107122
6	0	6.735533	0.292608	0.707166
6	0	6.792061	1.297026	-0.322292
8	0	7.864247	-0.021819	1.365146
8	0	5.673957	1.583491	-1.003222

7	0	7.819417	1.999321	-0.697259
6	0	7.419921	-0.960479	2.217683
6	0	6.115223	2.534816	-1.848680
7	0	6.152020	-1.203179	2.103532
7	0	7.375051	2.813631	-1.698512
6	0	8.359155	-1.567158	3.125702
8	0	7.916489	-2.508238	3.976863
6	0	9.044999	-2.809897	4.623485
7	0	9.628039	-1.321313	3.242869
7	0	10.080384	-2.150811	4.241003
7	0	8.980701	-3.827174	5.666574
8	0	7.892721	-4.318261	5.861323
8	0	10.021423	-4.069914	6.224501
6	0	5.218423	3.102370	-2.775213
8	0	5.091420	0.915526	-4.432606
6	0	4.413097	1.729446	-4.963349
7	0	4.480065	3.600014	-3.522954
7	0	3.865242	2.876283	-5.045272
7	0	3.654165	1.271922	-6.526067
8	0	4.364191	1.439857	-7.465665
8	0	2.623702	0.690524	-6.401407

Reaction: CN2O3 loss (step 2)
Structure: C7N8O5 (product)
Meth**o**d: M06/6-31+G(2df,p)

7	0	-0.928895	-0.252951	1.215543
6	0	0.114374	0.422033	0.848133
6	0	0.189628	1.462530	-0.144682
8	0	1.235438	0.071531	1.501482
8	0	-0.931752	1.810949	-0.795557
7	0	1.231095	2.138914	-0.514425
6	0	0.776539	-0.894758	2.315334
6	0	-0.475808	2.781164	-1.614239
7	0	-0.491759	-1.121579	2.183518
7	0	0.793425	3.006598	-1.481415
6	0	1.703636	-1.544060	3.206117
8	0	1.244597	-2.510567	4.019795
6	0	2.365349	-2.849256	4.661828
7	0	2.974823	-1.318242	3.340155
7	0	3.410797	-2.189196	4.310039
7	0	2.282540	-3.903269	5.665444
8	0	1.187878	-4.389689	5.834912
8	0	3.316490	-4.179054	6.221463
6	0	-1.386003	3.422121	-2.491667
7	0	-2.126709	3.945275	-3.207454

Decomposition of PHE-2

Structure: Ground state equilibrium
Meth**o**d: M06/6-31+G(2df,p)

6	0	-0.643372	1.252860	0.080932

8	0	-2.587976	2.026064	0.328049
6	0	0.462541	0.311284	-0.001916
6	0	1.536673	-1.435381	0.013206
7	0	-1.868077	0.857377	0.337824
8	0	2.403881	-0.457883	-0.248408
7	0	1.685225	0.705970	-0.257968
7	0	0.318470	-1.035447	0.177368
6	0	2.045564	-2.791312	0.080919
6	0	3.119696	-4.537977	0.096044
8	0	1.178356	-3.768811	0.342530
7	0	3.263768	-3.191245	-0.083239
7	0	1.897011	-4.932664	0.352091
6	0	4.225610	-5.479552	0.013198
8	0	6.170214	-6.252756	-0.233921
7	0	5.450314	-5.084070	-0.243702
7	0	-0.499894	2.602595	-0.098848
6	0	5.295729	-7.207042	0.026708
7	0	4.082135	-6.829286	0.192990
7	0	5.806088	-8.583288	0.096418
8	0	4.987294	-9.433299	0.337825
8	0	6.991839	-8.716474	-0.095621
6	0	-1.713488	2.980351	0.067432
7	0	-2.223845	4.356598	-0.002269
8	0	-1.405048	5.206611	-0.243659
8	0	-3.409598	4.489784	0.189760

Reaction: CONO isomerization
Structure: Transition State
Method: M06/6-31+G(2df,p)

6	0	-0.604135	1.288649	-0.033967
8	0	-2.566884	2.084247	0.067496
6	0	0.500856	0.341433	-0.056674
6	0	1.563482	-1.413868	-0.019434
7	0	-1.836058	0.871706	0.091382
8	0	2.456122	-0.434454	-0.157238
7	0	1.744407	0.735658	-0.181867
7	0	0.337606	-1.012396	0.049561
6	0	2.058179	-2.775632	0.035742
6	0	3.118613	-4.530733	0.073500
8	0	1.166788	-3.756927	0.174745
7	0	3.284742	-3.179246	-0.033588
7	0	1.876280	-4.926272	0.199701
6	0	4.223267	-5.477105	0.051546
8	0	6.179298	-6.256170	-0.049382
7	0	5.468369	-5.081743	-0.074735
7	0	-0.417139	2.639961	-0.144775
6	0	5.280027	-7.212864	0.088409
7	0	4.058093	-6.832406	0.158847
7	0	5.775594	-8.594851	0.145250
8	0	4.934346	-9.448313	0.269164
8	0	6.973856	-8.729677	0.061822

6	0	-1.650861	3.023250	-0.080952
7	0	-2.096603	4.477069	0.363755
8	0	-2.175253	4.315889	-0.918701
8	0	-2.223437	5.490913	0.936829

Reaction: CONO isomerization
Structure: CONO isomer of LLM-191 (product)
Meth**o**d: M06/6-31+G(2df,p)

6	0	-2.241862	3.431408	-0.145811
8	0	-4.168808	4.253653	0.029457
6	0	-1.161755	2.456875	-0.188106
6	0	-0.141038	0.676168	-0.126403
7	0	-3.475979	3.059729	0.083599
8	0	0.764655	1.621097	-0.371121
7	0	0.080998	2.808798	-0.411605
7	0	-1.349702	1.114155	-0.001257
6	0	0.320945	-0.694835	-0.031429
6	0	1.334493	-2.476904	0.032171
8	0	-0.585404	-1.641273	0.214048
7	0	1.529512	-1.138358	-0.155773
7	0	0.092778	-2.828546	0.256036
6	0	2.409373	-3.456345	-0.008461
8	0	4.332715	-4.300325	-0.190207
7	0	3.654246	-3.107093	-0.234213
7	0	-2.047489	4.769572	-0.328180
6	0	3.418056	-5.219862	0.055797
7	0	2.214261	-4.798556	0.182418
7	0	3.877420	-6.611683	0.156628
8	0	3.022899	-7.430429	0.382505
8	0	5.063182	-6.788877	0.002696
6	0	-3.261079	5.207791	-0.212193
7	0	-4.809373	6.784690	0.733681
8	0	-3.681246	6.440033	-0.337317
8	0	-5.218025	7.811735	0.507051

Reaction: NO2 loss
Structure: C8N9O6 radical
Meth**o**d: M06/6-31+G(2df,p)

6	0	-0.648447	1.250294	0.082518
8	0	-2.594635	2.048452	0.326416
6	0	0.458746	0.310558	-0.000338
6	0	1.535984	-1.435936	0.014734
7	0	-1.866337	0.845251	0.339588
8	0	2.402641	-0.458591	-0.247361
7	0	1.681739	0.705383	-0.256881
7	0	0.317804	-1.037771	0.179219
6	0	2.045709	-2.791586	0.082464
6	0	3.120409	-4.538200	0.096991
8	0	1.179422	-3.769879	0.345277
7	0	3.264053	-3.191765	-0.082801
7	0	1.898380	-4.933595	0.354441

6	0	4.226373	-5.479609	0.013114
8	0	6.170997	-6.253367	-0.236142
7	0	5.450924	-5.084416	-0.245311
7	0	-0.495908	2.609005	-0.100721
6	0	5.296650	-7.207292	0.025716
7	0	4.083328	-6.829560	0.193358
7	0	5.806884	-8.583435	0.095099
8	0	4.988583	-9.433606	0.337918
8	0	6.992421	-8.717104	-0.098584
6	0	-1.707305	2.971736	0.066547

Reaction: Central Ring Cleavage
Structure: Transition state
Method: M06/6-31+G(2df,p)

6	0	-0.064276	1.879184	-0.047149
8	0	-1.286851	3.174460	1.080818
6	0	0.673328	0.735040	-0.467887
6	0	1.215406	-1.656936	0.374690
7	0	-0.745874	1.909012	1.078153
8	0	1.985631	-0.680856	-1.679762
7	0	1.373149	0.314093	-1.357433
7	0	0.589656	-0.738420	0.742359
6	0	1.907770	-2.868669	0.121622
6	0	3.183625	-4.468798	0.018394
8	0	1.351802	-3.744666	-0.719934
7	0	3.038235	-3.250588	0.620738
7	0	2.208624	-4.811745	-0.784505
6	0	4.329582	-5.336486	0.242880
8	0	6.167580	-6.060880	0.976187
7	0	5.309587	-4.991490	1.044636
7	0	-0.116891	3.034480	-0.786522
6	0	5.602524	-6.917435	0.145303
7	0	4.476470	-6.560690	-0.352456
7	0	6.320267	-8.173172	-0.113656
8	0	5.776503	-8.941203	-0.865809
8	0	7.378974	-8.302780	0.454773
6	0	-0.869917	3.745971	-0.029979
7	0	-1.308290	5.126464	-0.282193
8	0	-0.905225	5.624871	-1.302240
8	0	-2.025380	5.613754	0.559339

Reaction: Central Ring Cleavage
Structure: C6N6O4 (product)
Method: M06/6-31+G(2df,p)

6	0	-0.993337	-0.122106	0.782209
7	0	-1.599283	0.819031	1.065967
6	0	-0.251624	-1.282982	0.427737
6	0	1.066042	-2.839155	0.201309
8	0	-0.731123	-2.053266	-0.554450
7	0	0.855676	-1.708608	0.940086
7	0	0.149682	-3.087258	-0.700902

6	0	2.214011	-3.713368	0.387876
8	0	4.014362	-4.503693	1.143870
7	0	3.131177	-3.463972	1.292780
6	0	3.524650	-5.250625	0.171215
7	0	2.426372	-4.845589	-0.351543
7	0	4.285364	-6.451600	-0.200566
8	0	3.817892	-7.110492	-1.094367
8	0	5.297774	-6.650811	0.428803

Reaction: Central Ring Cleavage
Structure: C3N4O4 (product)
Meth**o**d: M06/6-31+G(2df,p)
E0 = -633.645785459 Hartree

6	0	-2.181271	3.934253	-0.261976
8	0	-3.349993	5.102367	1.055579
6	0	-1.440741	2.859799	-0.788315
7	0	-2.739443	3.878293	0.932132
8	0	-0.197248	1.091984	-1.702555
7	0	-0.825671	1.987652	-1.242480
7	0	-2.386463	5.117912	-0.931534
6	0	-3.091916	5.746502	-0.065655
7	0	-3.637894	7.105617	-0.198180
8	0	-3.389408	7.670157	-1.232982
8	0	-4.276802	7.511271	0.743643

Reaction: Central Ring Opening
Structure: Transition state
Meth**o**d: M06/6-31+G(2df,p)

6	0	-0.578525	1.148390	-0.004559
8	0	-2.631545	0.989909	0.384235
6	0	0.805534	0.777998	-0.277185
6	0	2.448028	-0.976583	-0.288404
7	0	-1.512171	0.242525	0.144649
8	0	3.479413	-0.348033	-0.187524
7	0	1.831935	1.457873	-0.457282
7	0	1.190701	-0.530023	-0.477405
6	0	2.477768	-2.474459	-0.204253
6	0	2.963665	-4.460014	-0.015598
8	0	1.348424	-3.169809	-0.370626
7	0	3.514292	-3.211807	0.018638
7	0	1.674061	-4.491110	-0.246718
6	0	3.730593	-5.680228	0.184093
8	0	5.347892	-6.984965	0.543858
7	0	5.021816	-5.656270	0.418835
7	0	-0.992183	2.443828	0.117982
6	0	4.218445	-7.645267	0.369934
7	0	3.177094	-6.933004	0.144650
7	0	4.279362	-9.110531	0.453327
8	0	3.235261	-9.689068	0.288487
8	0	5.369307	-9.582388	0.678518
6	0	-2.239535	2.253396	0.350916

7	0	-3.263845	3.283338	0.581751
8	0	-2.872236	4.421160	0.544676
8	0	-4.382078	2.874695	0.782564

Reaction: Central Ring Opening
Structure: Product
Method: M06/6-31+G(2df,p)

6	0	-1.632262	3.291547	-0.441199
8	0	-3.250106	2.457867	0.607053
6	0	-0.378396	3.344023	-1.140179
6	0	1.441868	1.849993	-0.753581
7	0	-2.082933	2.131321	-0.020818
8	0	2.235318	2.458123	-0.105456
7	0	0.570846	4.015768	-1.574387
7	0	0.516378	2.418184	-1.682905
6	0	1.350904	0.361774	-0.737319
6	0	1.523091	-1.652699	-0.381037
8	0	0.423883	-0.245476	-1.483887
7	0	2.064250	-0.450777	-0.029537
7	0	0.539135	-1.584262	-1.245370
6	0	1.983031	-2.926747	0.150366
8	0	3.082894	-4.348496	1.251993
7	0	2.970403	-3.000995	1.011867
7	0	-2.419697	4.365812	-0.139235
6	0	2.153374	-4.920346	0.509480
7	0	1.431970	-4.131569	-0.197741
7	0	2.049022	-6.384188	0.576297
8	0	1.185834	-6.879493	-0.102934
8	0	2.838960	-6.937322	1.305045
6	0	-3.368042	3.771849	0.487573
7	0	-4.561985	4.395372	1.081366
8	0	-4.646377	5.587927	0.943088
8	0	-5.322312	3.642435	1.640469

Reaction: CN2O2 loss
Structure: Transition state
Method: M06/6-31+G(2df,p)

6	0	-0.850498	0.854744	0.105242
8	0	-2.760539	2.087525	0.102782
6	0	0.111666	-0.195634	0.129266
6	0	0.921689	-2.078644	0.203459
7	0	-2.022055	1.123801	0.129282
8	0	1.941778	-1.229986	0.122936
7	0	1.403996	0.029956	0.073138
7	0	-0.243263	-1.515772	0.212673
6	0	1.220631	-3.496031	0.269901
6	0	2.026381	-5.380007	0.343657
8	0	0.196270	-4.344435	0.352334
7	0	2.381800	-4.063390	0.259536
7	0	0.736255	-5.600408	0.401450
6	0	2.990379	-6.469302	0.368480

8	0	4.823344	-7.508329	0.358913
7	0	4.282513	-6.247826	0.309168
7	0	-0.096939	2.681991	-0.014921
6	0	3.795834	-8.333423	0.441827
7	0	2.635444	-7.788794	0.454080
7	0	4.093778	-9.770831	0.510382
8	0	3.137849	-10.500044	0.585292
8	0	5.264776	-10.068508	0.484446
6	0	-1.002616	3.428723	-0.024693
7	0	-1.762190	4.628084	-0.062605
8	0	-2.075550	5.014644	-1.163223
8	0	-2.008289	5.125752	1.010119

Reaction: CN2O2 loss
Structure: C7N8O6 (product)
Meth**o**d: M06/6-31+G(2df,p)

6	0	-2.149293	3.306397	-0.107408
8	0	-3.797251	4.978351	-0.143249
6	0	-1.181026	2.283795	-0.084726
6	0	-0.307802	0.422989	-0.012733
7	0	-2.965194	4.130024	-0.124970
8	0	0.686987	1.302993	-0.096074
7	0	0.108893	2.543184	-0.144170
7	0	-1.488279	0.948789	-0.000343
6	0	0.038214	-0.983805	0.052319
6	0	0.905884	-2.840445	0.122705
8	0	-0.957184	-1.865993	0.136917
7	0	1.217523	-1.512961	0.038583
7	0	-0.375972	-3.103637	0.183744
6	0	1.905296	-3.897412	0.144139
8	0	3.771502	-4.876068	0.129646
7	0	3.189451	-3.633759	0.082742
6	0	2.771675	-5.734332	0.213257
7	0	1.594117	-5.228125	0.228460
7	0	3.116671	-7.161174	0.279101
8	0	2.185392	-7.921664	0.354159
8	0	4.296785	-7.420451	0.251079

Reaction: CN2O3 loss (step 1)
Structure: Transition state
Meth**o**d: M06/6-31+G(2df,p)

6	0	-0.891842	1.073944	-0.061300
8	0	-2.916220	3.226879	-0.567814
6	0	0.242458	0.164699	-0.174456
6	0	1.381220	-1.532917	-0.103771
7	0	-2.051604	0.899547	0.334405
8	0	2.164349	-0.558887	-0.574771
7	0	1.402298	0.570622	-0.620781
7	0	0.174092	-1.153340	0.165642
6	0	1.958204	-2.854426	0.043681
6	0	3.108893	-4.549614	0.108325

8	0	1.176420	-3.824548	0.514942
7	0	3.164738	-3.226415	-0.229726
7	0	1.946189	-4.954349	0.557169
6	0	4.240805	-5.455432	-0.013357
8	0	6.175360	-6.181366	-0.421368
7	0	5.403872	-5.047680	-0.463884
7	0	-0.724193	2.434657	-0.370809
6	0	5.387203	-7.131529	0.047633
7	0	4.185827	-6.780408	0.325230
7	0	5.969102	-8.472858	0.197831
8	0	5.226415	-9.319499	0.625049
8	0	7.128916	-8.583026	-0.122842
6	0	-1.728951	3.221178	-0.646109
7	0	-1.045754	4.541696	-1.275801
8	0	-0.685025	5.357177	-0.473481
8	0	-1.050050	4.591867	-2.473868

Reaction: CN2O3 loss (Step 1)
Structure: Product
Meth**o**d: M06/6-31+G(2df,p)

6	0	-3.290379	2.732553	0.742703
8	0	-4.973565	4.629104	-1.017597
6	0	-2.068671	2.003486	0.540829
6	0	-0.731477	0.466382	0.353159
7	0	-4.518942	2.672360	0.922169
8	0	-0.048593	1.600052	0.164432
7	0	-0.939562	2.621377	0.290283
7	0	-1.990348	0.641778	0.590080
6	0	-0.002459	-0.784186	0.273259
6	0	1.346755	-2.316152	0.088287
8	0	-0.683973	-1.913021	0.461630
7	0	1.256336	-0.953152	0.037709
7	0	0.218102	-2.933492	0.337695
6	0	2.589433	-3.044622	-0.115748
8	0	4.622525	-3.449099	-0.488139
7	0	3.718720	-2.424399	-0.364512
7	0	-3.722102	4.054688	0.876068
6	0	3.931502	-4.558599	-0.299788
7	0	2.679894	-4.409380	-0.065573
7	0	4.666763	-5.828822	-0.378666
8	0	4.010221	-6.823850	-0.206174
8	0	5.849811	-5.739484	-0.607787
6	0	-4.076089	4.768738	-0.270707
7	0	-3.107742	5.980507	-0.408590
8	0	-1.961269	5.762684	-0.091034
8	0	-3.577831	6.988751	-0.860833

Reaction: CN2O3 loss (step 2)
Structure: Transition state
Meth**o**d: M06/6-31+G(2df,p)

6	0	-1.080530	0.808787	0.257699
8	0	-3.119667	3.236517	0.352531

6	0	0.169675	0.073235	0.097998
6	0	1.516660	-1.466066	0.027215
7	0	-2.219030	0.454551	0.538427
8	0	2.189777	-0.349957	-0.261707
7	0	1.288741	0.673783	-0.213572
7	0	0.258733	-1.277747	0.261134
6	0	2.251921	-2.715183	0.044617
6	0	3.608235	-4.250872	-0.024530
8	0	1.578644	-3.828506	0.330922
7	0	3.510060	-2.897390	-0.186527
7	0	2.485401	-4.851457	0.284212
6	0	4.853377	-4.987492	-0.177709
8	0	6.886285	-5.411690	-0.531129
7	0	5.977491	-4.384557	-0.485717
7	0	-0.989075	2.245958	0.050188
6	0	6.202667	-6.504972	-0.246314
7	0	4.952055	-6.343124	-0.015620
7	0	6.944267	-7.773619	-0.225651
8	0	6.294943	-8.754425	0.033948
8	0	8.125099	-7.697864	-0.471017
6	0	-1.978938	3.036000	0.146846
7	0	-1.061884	4.533186	-0.238591
8	0	-0.656595	5.107828	0.722448
8	0	-1.089124	4.828422	-1.391911

Reaction: CN2O3 loss (Step 2)
Structure: C7N8O5 (product)
Meth**o**d: M06/6-31+G(2df,p)

6	0	-3.492713	2.290678	0.453074
6	0	-2.242967	1.626883	0.277669
6	0	-0.813690	0.160573	0.169291
7	0	-4.507748	2.821852	0.596573
8	0	-0.201979	1.311514	-0.108773
7	0	-1.153485	2.287760	-0.036607
7	0	-2.077348	0.277455	0.418731
6	0	-0.015965	-1.050030	0.160228
6	0	1.415073	-2.514089	0.052906
8	0	-0.628673	-2.200384	0.437130
7	0	1.247123	-1.165243	-0.087532
7	0	0.327926	-3.175524	0.364869
6	0	2.693898	-3.184618	-0.125366
8	0	4.741251	-3.500339	-0.509086
7	0	3.782334	-2.521156	-0.437443
6	0	4.117114	-4.630798	-0.232573
7	0	2.862928	-4.535793	0.015292
7	0	4.921974	-5.860267	-0.239648
8	0	4.326730	-6.876475	0.014380
8	0	6.094260	-5.721786	-0.499232

Decomposition of PHE-3

Structure: Ground state equilibrium
Method: M06/6-31+G(2df,p)

6	0	-0.776409	1.136452	0.117466
6	0	0.368377	0.254309	0.020818
6	0	1.509647	-1.445767	0.018967
7	0	-2.007142	0.813360	0.367736
8	0	2.336933	-0.432802	-0.241037
7	0	1.573441	0.700240	-0.239306
7	0	0.277150	-1.096852	0.192307
6	0	2.072589	-2.780927	0.075172
6	0	3.213860	-4.481003	0.073315
8	0	1.245307	-3.793891	0.335195
7	0	3.305084	-3.129843	-0.098184
7	0	2.008800	-4.926932	0.333460
6	0	4.358644	-5.363146	-0.023349
7	0	5.589367	-5.040058	-0.273674
6	0	5.431216	-7.129590	-0.005891
7	0	5.665795	-8.562676	0.118234
8	0	4.694385	-9.240878	0.365018
8	0	6.805990	-8.923119	-0.038430
6	0	-1.848977	2.902899	0.100015
7	0	-2.083547	4.335990	-0.024075
8	0	-1.112120	5.014200	-0.270768
8	0	-3.223752	4.696427	0.132525
7	0	6.299927	-6.217913	-0.261228
8	0	4.183593	-6.685475	0.159162
8	0	-0.601348	2.458786	-0.065001
7	0	-2.717699	1.991217	0.355294

Reaction: CONO isomerization
Structure: Transition State
Method: M06/6-31+G(2df,p)

6	0	-0.667829	1.222380	0.171527
6	0	0.453492	0.326037	0.042863
6	0	1.569041	-1.393937	0.026139
7	0	-1.883791	0.953158	0.491163
8	0	2.401550	-0.404603	-0.291908
7	0	1.654836	0.744944	-0.281152
7	0	0.351557	-1.022532	0.246680
6	0	2.110012	-2.738169	0.086459
6	0	3.218331	-4.460409	0.070717
8	0	1.277347	-3.730029	0.405429
7	0	3.326988	-3.115673	-0.134208
7	0	2.018593	-4.877613	0.394317
6	0	4.340173	-5.367527	-0.058149
7	0	5.564628	-5.076260	-0.371333
6	0	5.376790	-7.155739	-0.050303
7	0	5.587777	-8.590238	0.094659
8	0	4.615578	-9.242554	0.400744

8	0	6.711826	-8.978513	-0.106045
6	0	-1.682254	3.035506	0.186993
7	0	-2.007950	4.425520	-0.410922
8	0	-1.754733	4.514850	0.864224
8	0	-2.666363	5.173608	-1.034005
7	0	6.251112	-6.268484	-0.365059
8	0	4.147513	-6.681928	0.161383
8	0	-0.463023	2.563540	-0.062080
7	0	-2.578850	2.149246	0.514447

Reaction: CONO isomerization
Structure: CONO isomer of PHE-3 (product)
Meth**o**d: M06/6-31+G(2df,p)

6	0	-2.329649	3.331146	0.168120
6	0	-1.217285	2.414657	0.063598
6	0	-0.135771	0.671948	0.035421
7	0	-3.566181	3.049753	0.409222
8	0	0.732516	1.654251	-0.195150
7	0	0.008159	2.818694	-0.176650
7	0	-1.355736	1.060812	0.204812
6	0	0.373699	-0.685327	0.068984
6	0	1.445171	-2.430841	0.041996
8	0	-0.495478	-1.670442	0.300710
7	0	1.593062	-1.082074	-0.100667
7	0	0.221194	-2.833442	0.282227
6	0	2.552980	-3.358083	-0.063036
7	0	3.799017	-3.083982	-0.297065
6	0	3.548939	-5.169458	-0.071940
7	0	3.720804	-6.612894	0.025714
8	0	2.719483	-7.254017	0.251293
8	0	4.845734	-7.019631	-0.128815
6	0	-3.339619	5.162166	0.206623
7	0	-4.835204	6.763343	-0.736009
8	0	-3.491687	6.450361	0.120534
8	0	-5.120802	7.840930	-0.586273
7	0	4.458249	-4.291507	-0.302220
8	0	2.320411	-4.675395	0.091755
8	0	-2.104332	4.656194	0.014094
7	0	-4.235621	4.251517	0.447941

Reaction: NO2 loss
Structure: C8N9O6 radical
Meth**o**d: M06/6-31+G(2df,p)

6	0	-0.777506	1.132789	0.117971
6	0	0.367934	0.253939	0.021122
6	0	1.513412	-1.445477	0.018737
7	0	-2.003140	0.811672	0.367574
8	0	2.340127	-0.433759	-0.241286
7	0	1.573248	0.700395	-0.239291
7	0	0.280646	-1.099016	0.192446
6	0	2.076460	-2.780667	0.075009

6	0	3.217040	-4.481585	0.073242
8	0	1.249262	-3.794034	0.335284
7	0	3.309037	-3.130851	-0.098424
7	0	2.012154	-4.927455	0.333607
6	0	4.361094	-5.364711	-0.023409
7	0	5.592478	-5.043481	-0.273689
6	0	5.431557	-7.132749	-0.005797
7	0	5.664397	-8.565802	0.118334
8	0	4.692363	-9.243269	0.365055
8	0	6.804221	-8.927990	-0.038197
6	0	-1.849086	2.895902	0.099358
7	0	6.301498	-6.222297	-0.261122
8	0	4.184605	-6.687032	0.159143
8	0	-0.599805	2.468738	-0.067635
7	0	-2.731540	2.012129	0.354695

Reaction: Central Ring Cleavage
Structure: Transition state
Meth**o**d: M06/6-31+G(2df,p)

6	0	-0.557450	1.765023	-0.131431
6	0	0.373899	0.764021	0.247811
6	0	0.769860	-1.763086	-0.188873
7	0	-1.606254	1.636999	-0.890160
8	0	2.145274	-0.309884	1.203507
7	0	1.372228	0.570284	0.900212
7	0	-0.010797	-0.946796	-0.493168
6	0	1.608212	-2.878472	0.065240
6	0	2.969759	-4.406075	0.062584
8	0	1.461323	-3.520351	1.228703
7	0	2.518639	-3.373539	-0.708588
7	0	2.373536	-4.540071	1.221027
6	0	4.030045	-5.295029	-0.366159
7	0	4.684797	-5.265707	-1.485073
6	0	5.381698	-6.855770	-0.281525
7	0	6.076647	-8.007975	0.278467
8	0	5.719801	-8.360338	1.379726
8	0	6.936238	-8.490422	-0.416115
6	0	-1.424757	3.641690	-0.235967
7	0	-1.588520	5.063458	0.026376
8	0	-0.752587	5.572031	0.739633
8	0	-2.541205	5.588300	-0.494583
7	0	5.583255	-6.305720	-1.425078
8	0	4.423524	-6.287915	0.453349
8	0	-0.378074	3.021008	0.323744
7	0	-2.174801	2.886929	-0.953445

Reaction: Central Ring Cleavage
Structure: C5N6O4 (product)
Meth**o**d: M06/6-31+G(2df,p)

6	0	-1.272474	-0.381853	-0.449262
7	0	-2.024873	0.458441	-0.696398

6	0	-0.348713	-1.417412	-0.137566
6	0	1.107051	-2.857162	-0.057565
8	0	-0.396705	-1.945555	1.091209
7	0	0.557677	-1.934015	-0.900301
7	0	0.574384	-2.903230	1.138825
6	0	2.198394	-3.724614	-0.451051
7	0	2.799967	-3.770461	-1.598819
6	0	3.643249	-5.192361	-0.283507
7	0	4.430110	-6.243046	0.349852
8	0	4.144176	-6.503154	1.496644
8	0	5.285480	-6.743949	-0.337011
7	0	3.760716	-4.748202	-1.483495
8	0	2.686309	-4.607874	0.440126

Reaction: Central Ring Cleavage
Structure: C3N4O4 (product)
Meth**o**d: M06/6-31+G(2df,p)
E0 = -633.645785459 Hartree

6	0	-2.283285	3.880263	0.011772
6	0	-1.314876	2.984886	0.472360
7	0	-3.267953	3.650467	-0.812591
8	0	0.273719	1.418050	1.194899
7	0	-0.530158	2.206104	0.827639
6	0	-3.301205	5.674988	-0.206866
7	0	-3.608704	7.083651	-0.002936
8	0	-2.874111	7.684216	0.749148
8	0	-4.564277	7.506515	-0.605023
8	0	-2.250399	5.166010	0.437901
7	0	-3.934779	4.840639	-0.951360

Reaction: Central Ring Opening
Structure: Transition state
Meth**o**d: M06/6-31+G(2df,p)

6	0	-0.678794	1.000143	0.012128
6	0	0.712663	0.707227	-0.282857
6	0	2.415341	-0.977544	-0.306332
7	0	-1.634441	0.153917	0.215545
8	0	3.418848	-0.306096	-0.205657
7	0	1.707259	1.431953	-0.474500
7	0	1.140467	-0.583786	-0.498254
6	0	2.507231	-2.472782	-0.218901
6	0	3.071010	-4.432401	-0.010727
8	0	1.417558	-3.216597	-0.437374
7	0	3.565034	-3.163015	0.049953
7	0	1.795239	-4.520862	-0.301213
6	0	3.886746	-5.606473	0.223396
7	0	5.148158	-5.653705	0.522477
6	0	4.360810	-7.610606	0.407253
7	0	4.145447	-9.051096	0.408323
8	0	3.021002	-9.421761	0.156686
8	0	5.112036	-9.727240	0.660498

6	0	-2.359703	2.133322	0.384436
7	0	-3.164581	3.339261	0.566002
8	0	-2.576257	4.388179	0.442858
8	0	-4.327497	3.154951	0.818888
8	0	-1.064522	2.285479	0.103638
7	0	-2.755454	0.911825	0.464014
8	0	3.318318	-6.824470	0.133300
7	0	5.459558	-6.988277	0.643979

Reaction: Central Ring Opening
Structure: Product
Method: M06/6-31+G(2df,p)

6	0	-1.679510	3.126593	-0.431706
6	0	-0.457719	3.244181	-1.161304
6	0	1.423291	1.837338	-0.773381
7	0	-2.146297	2.020986	0.063538
8	0	2.206988	2.488688	-0.157929
7	0	0.454294	3.951094	-1.624979
7	0	0.465535	2.352123	-1.705054
6	0	1.373716	0.348574	-0.711772
6	0	1.607544	-1.646210	-0.302140
8	0	0.453464	-0.304893	-1.428173
7	0	2.120144	-0.422117	0.008522
7	0	0.609828	-1.630915	-1.154552
6	0	2.116433	-2.879783	0.261773
7	0	3.085570	-3.025888	1.111374
6	0	2.276790	-4.911485	0.608427
7	0	1.962486	-6.328481	0.483288
8	0	1.056227	-6.608428	-0.268501
8	0	2.639612	-7.077152	1.143389
6	0	-3.426070	3.630803	0.539699
7	0	-4.503608	4.491929	1.024683
8	0	-4.418720	5.659934	0.725958
8	0	-5.358124	3.940261	1.669444
8	0	-2.446415	4.197635	-0.165912
7	0	-3.307087	2.360581	0.711612
8	0	1.552450	-4.046865	-0.104155
7	0	3.189125	-4.378623	1.339464

Reaction: CN2O2 loss
Structure: Transition state
Method: M06/6-31+G(2df,p)

6	0	-0.410243	1.633258	0.282625
6	0	0.692978	0.562840	0.540951
6	0	1.697909	-1.207256	0.385986
7	0	-0.642831	1.678163	1.539302
8	0	2.593004	-0.292163	0.767273
7	0	1.913189	0.890124	0.879670
7	0	0.498925	-0.748300	0.232398
6	0	2.160065	-2.568566	0.199208
6	0	3.168770	-4.343021	0.036940

8	0	1.262070	-3.483745	-0.167337
7	0	3.359860	-3.026884	0.344382
7	0	1.937256	-4.666562	-0.274923
6	0	4.241305	-5.316319	0.051055
7	0	5.489687	-5.116758	0.339828
6	0	5.175040	-7.150106	-0.138959
7	0	5.300505	-8.577297	-0.406484
8	0	4.283257	-9.149644	-0.725712
8	0	6.407413	-9.039082	-0.281409
6	0	-2.333467	3.322083	0.375340
7	0	-2.808396	3.896218	-0.852380
8	0	-2.253377	4.907990	-1.193818
8	0	-3.709685	3.299639	-1.381915
7	0	6.107737	-6.339194	0.212269
8	0	3.967686	-6.595977	-0.265212
8	0	-0.746611	2.055133	-0.803155
7	0	-2.097722	2.979091	1.462033

Reaction: CN2O2 loss
Structure: C7N8O6 (product)
Meth**o**d: M06/6-31+G(2df,p)

6	0	-2.517437	3.770065	-0.060015
6	0	-0.542451	2.622351	0.590476
6	0	0.366710	0.787494	0.436089
7	0	-1.436178	3.635962	0.467806
8	0	1.189659	1.554638	1.139165
7	0	0.584269	2.785226	1.245035
7	0	-0.724063	1.371957	0.060115
6	0	0.771044	-0.580404	0.175829
6	0	1.666729	-2.415518	0.013570
8	0	-0.060129	-1.350229	-0.529405
7	0	1.859303	-1.173729	0.544917
7	0	0.539442	-2.573776	-0.636256
6	0	2.631632	-3.486923	0.152183
7	0	3.774964	-3.452059	0.763548
6	0	3.455804	-5.370517	-0.061181
7	0	3.547841	-6.760463	-0.488384
8	0	2.609031	-7.185137	-1.123116
8	0	4.552081	-7.344304	-0.164055
7	0	4.320194	-4.706889	0.619310
8	0	2.362097	-4.685303	-0.399805
8	0	-3.547855	4.017472	-0.521554

Reaction: CN2O3 loss (Step 1)
Structure: Transition state
Meth**o**d: M06/6-31+G(2df,p)

6	0	-1.479576	0.562262	0.731267
6	0	-0.528185	-0.486334	0.827520
6	0	0.349161	-2.334852	0.724527
7	0	-2.524467	1.131300	0.820170
8	0	1.292552	-1.482167	1.129032

7	0	0.708337	-0.255440	1.210627
7	0	-0.803322	-1.788688	0.511357
6	0	0.716541	-3.729014	0.570207
6	0	1.598571	-5.573794	0.472344
8	0	-0.227161	-4.578368	0.164132
7	0	1.869951	-4.271541	0.780805
7	0	0.363695	-5.808835	0.099665
6	0	2.595288	-6.621886	0.548996
7	0	3.837334	-6.508877	0.903465
6	0	3.403516	-8.519070	0.419788
7	0	3.439857	-9.954583	0.167659
8	0	2.401963	-10.455099	-0.201393
8	0	4.502576	-10.492593	0.354062
6	0	-1.796717	2.828003	-0.152605
7	0	-1.996878	4.209029	-0.696205
8	0	-2.072379	4.290305	-1.896622
8	0	-2.042987	5.093081	0.121437
7	0	4.371931	-7.773399	0.816228
8	0	2.247372	-7.881276	0.225603
8	0	-0.714432	2.280443	-0.265807
7	0	-2.915030	2.328095	0.421485

Reaction: CN2O3 loss (Step 1)
Structure: Product
Meth**o**d: M06/6-31+G(2df,p)

6	0	-2.662700	2.686947	0.144779
6	0	-1.712203	1.755064	-0.324386
6	0	-0.288833	0.280808	-0.351014
7	0	-3.432640	3.436377	0.569992
8	0	-0.491375	0.639019	-1.617765
7	0	-1.439260	1.621256	-1.604685
7	0	-1.008496	0.927510	0.507557
6	0	0.684875	-0.760731	-0.086631
6	0	2.106470	-2.233598	-0.110999
8	0	0.884076	-1.115154	1.182871
7	0	1.404500	-1.408235	-0.942148
7	0	1.833046	-2.098110	1.164152
6	0	3.081485	-3.189469	-0.594294
7	0	3.431874	-3.410454	-1.822901
6	0	4.510177	-4.680468	-0.523910
7	0	5.396903	-5.670677	0.075341
8	0	5.349971	-5.764708	1.280676
8	0	6.084651	-6.292485	-0.695262
6	0	-4.910321	5.021948	0.254436
7	0	-5.890215	5.940370	1.062679
8	0	-5.924118	5.806229	2.261337
8	0	-6.527010	6.706587	0.387797
7	0	4.382775	-4.403260	-1.772087
8	0	3.731289	-3.966807	0.291747
8	0	-4.857783	5.121361	-0.925522
7	0	-4.247250	4.213761	1.137807

Reaction: CN2O3 loss (Step 2)
Structure: Transition state
Method: M06/6-31+G(2df,p)

6	0	-0.897865	0.729148	-0.666636
6	0	0.265437	-0.010882	-1.008772
6	0	1.944836	-1.169022	-0.866657
7	0	-1.864245	1.306978	-0.387719
8	0	1.807773	-0.843101	-2.155188
7	0	0.690756	-0.074821	-2.250288
7	0	1.021593	-0.690577	-0.098711
6	0	3.076376	-1.995117	-0.493854
6	0	4.761976	-3.148705	-0.360887
8	0	3.210569	-2.320991	0.791406
7	0	3.996567	-2.470486	-1.265912
7	0	4.335923	-3.090717	0.877806
6	0	5.955122	-3.879898	-0.734488
7	0	6.466218	-4.008365	-1.919137
6	0	7.641756	-5.051525	-0.507455
7	0	8.644812	-5.850497	0.186291
8	0	8.495359	-5.969290	1.381027
8	0	9.518905	-6.309712	-0.505543
6	0	-0.777151	3.247127	0.397749
7	0	-1.227018	4.851059	1.059619
8	0	-1.244536	4.889316	2.249328
8	0	-1.261992	5.712527	0.238741
7	0	7.588511	-4.788605	-1.764071
8	0	6.655388	-4.521809	0.218960
8	0	0.378400	3.012437	0.286319
7	0	-2.014579	2.957560	0.294043

Reaction: CN2O3 loss (Step 2)
Structure: C7N8O5 (product)
Method: M06/6-31+G(2df,p)

6	0	-4.126090	1.517144	-0.682514
6	0	-2.910034	0.838869	-0.989214
6	0	-1.175136	-0.235545	-0.791622
7	0	-5.109862	2.064554	-0.426524
8	0	-1.297842	0.055426	-2.085991
7	0	-2.452805	0.770728	-2.217699
7	0	-2.134470	0.215962	-0.051452
6	0	-0.016126	-1.000982	-0.375726
6	0	1.716510	-2.073845	-0.177388
8	0	0.104285	-1.291254	0.920198
7	0	0.943239	-1.452203	-1.114999
7	0	1.260974	-2.007090	1.050119
6	0	2.949996	-2.758433	-0.506006
7	0	3.497039	-2.889058	-1.674490
6	0	4.681462	-3.847418	-0.211093
7	0	5.701290	-4.584393	0.524507
8	0	5.528262	-4.683756	1.718118

8	0	6.612617	-5.018916	-0.135125
7	0	4.648791	-3.614126	-1.474234
8	0	3.654133	-3.347526	0.478676

Decomposition of TKX-55

Structure: Ground state equilibrium
Method: M06/6-31+G(2df,p)

7	0	5.868044	-0.202651	1.614805
6	0	6.761434	-0.221328	0.682287
6	0	6.635546	0.221325	-0.682267
8	0	7.942475	-0.733084	1.084337
8	0	5.454512	0.733095	-1.084318
7	0	7.528940	0.202645	-1.614784
6	0	7.679340	-1.023584	2.365366
6	0	5.717652	1.023603	-2.365346
7	0	6.476548	-0.740760	2.730762
6	0	8.713809	-1.645523	3.203938
6	0	4.683196	1.645538	-3.203925
7	0	6.920444	0.740767	-2.730736
6	0	8.613533	-2.991720	3.555431
6	0	9.788414	-0.940213	3.748225
6	0	3.608441	0.940283	-3.747989
6	0	4.783620	2.991664	-3.555653
7	0	7.546454	-3.839639	2.974465
6	0	9.499586	-3.613451	4.414126
7	0	9.966468	0.508407	3.475128
6	0	10.720182	-1.533074	4.581202
6	0	2.676665	1.533133	-4.580965
7	0	3.430245	-0.508275	-3.474674
6	0	3.897572	3.613367	-4.414373
7	0	5.850851	3.839548	-2.974916
8	0	7.167769	-4.768049	3.650527
8	0	7.165834	-3.557518	1.859964
1	0	9.377172	-4.657177	4.682273
6	0	10.551449	-2.864462	4.903098
8	0	9.054527	1.090686	2.932142
8	0	11.012828	1.001417	3.829299
1	0	11.549877	-0.959501	4.978751
1	0	1.846847	0.959610	-4.978329
6	0	2.845552	2.864442	-4.903108
8	0	2.383699	-1.001159	-3.828473
8	0	4.342269	-1.090636	-2.931916
1	0	4.020103	4.657029	-4.682714
8	0	6.231436	3.557647	-1.860348
8	0	6.229675	4.767728	-3.651218
7	0	11.530094	-3.510736	5.804689
7	0	1.866907	3.510697	-5.804710
8	0	11.351025	-4.681743	6.055551
8	0	12.432123	-2.818399	6.220122
8	0	0.964737	2.818417	-6.219928

8	0	2.046117	4.681635	-6.055796

Reaction: CONO isomerization
Structure: Transition State
Method: M06/6-31+G(2df,p)

7	0	6.496970	0.743096	1.682835
6	0	6.937201	0.020724	0.706748
6	0	6.553926	0.067020	-0.679479
8	0	7.858648	-0.887973	1.086989
8	0	5.636638	0.970591	-1.065986
7	0	6.970925	-0.683835	-1.648184
6	0	7.938894	-0.643444	2.401207
6	0	5.527975	0.716933	-2.384838
7	0	7.158696	0.298557	2.808344
6	0	8.824335	-1.455506	3.248696
6	0	4.609151	1.466386	-3.213041
7	0	6.284982	-0.268543	-2.760383
6	0	8.284981	-2.429251	4.089827
6	0	10.204263	-1.261301	3.328095
6	0	4.113923	0.874811	-4.395745
6	0	4.129958	2.744958	-2.926021
7	0	6.838658	-2.747427	4.037333
6	0	9.048263	-3.162462	4.978265
7	0	10.876329	-0.222409	2.506884
6	0	11.009791	-1.997088	4.178807
6	0	3.187329	1.516773	-5.215669
7	0	4.926828	-0.330359	-5.103437
6	0	3.192879	3.409059	-3.692038
7	0	4.697039	3.525718	-1.803669
8	0	6.342608	-3.171978	5.054885
8	0	6.277980	-2.589679	2.975106
1	0	8.591637	-3.897818	5.631754
6	0	10.410053	-2.935772	4.993309
8	0	10.171669	0.529090	1.870956
8	0	12.085150	-0.201630	2.542239
1	0	12.080237	-1.827689	4.210007
1	0	2.818107	1.047380	-6.120481
6	0	2.750189	2.767110	-4.834417
8	0	3.910228	-0.781734	-4.429709
8	0	5.364898	-0.854215	-6.062531
1	0	2.841194	4.397560	-3.423888
8	0	5.904635	3.606421	-1.759839
8	0	3.907278	4.060624	-1.061024
7	0	11.255009	-3.724314	5.917082
7	0	1.759348	3.450822	-5.694322
8	0	10.690939	-4.543391	6.607695
8	0	12.442256	-3.488424	5.908899
8	0	1.399455	2.866376	-6.693295
8	0	1.381724	4.544140	-5.334960

Reaction: CONO isomerization
Structure: CONO isomer of LLM-191 (product)
Meth**o**d: M06/6-31+G(2df,p)

Reaction: NO2 loss
Structure: C16H4N9O12 radical
Meth**o**d: M06/6-31+G(2df,p)

7	0	5.805111	-0.388499	1.578034
6	0	6.778027	-0.107307	0.775800
6	0	6.718457	0.565880	-0.494977
8	0	7.978514	-0.525120	1.225554
8	0	5.524949	0.989496	-0.944619
7	0	7.694001	0.830806	-1.304211
6	0	7.639182	-1.089859	2.391503
6	0	5.860034	1.557942	-2.122978
7	0	6.376862	-1.045679	2.648188
6	0	8.669801	-1.719099	3.230451
6	0	4.793957	2.078955	-2.956691
7	0	7.127730	1.479470	-2.373284
6	0	8.770468	-3.109200	3.292864
6	0	9.534459	-0.996120	4.053999
6	0	3.501669	1.624496	-2.813253
6	0	4.980570	2.985461	-4.009960
7	0	7.932460	-3.961226	2.416800
6	0	9.655262	-3.762531	4.129413
7	0	9.483145	0.487586	4.099555
6	0	10.458400	-1.609721	4.880962
6	0	2.421667	1.944379	-3.584358
6	0	3.953319	3.339540	-4.861723
7	0	6.273833	3.671465	-4.220993
8	0	7.674060	-5.068324	2.828537
8	0	7.601304	-3.495778	1.348571
1	0	9.692051	-4.845833	4.166072
6	0	10.497108	-2.988981	4.903255
8	0	8.586142	1.034685	3.497903
8	0	10.342942	1.039843	4.746399
1	0	11.122152	-1.018376	5.501720
1	0	1.421040	1.556614	-3.423661
6	0	2.689875	2.817619	-4.632896
1	0	4.126346	4.024269	-5.684602
8	0	6.737818	4.246534	-3.264087
8	0	6.726210	3.639074	-5.342611
7	0	11.471614	-3.662319	5.789959
7	0	1.587372	3.209512	-5.535165
8	0	11.477976	-4.872986	5.773970
8	0	12.184578	-2.949906	6.460269
8	0	0.497553	2.727739	-5.311453
8	0	1.852910	3.981838	-6.430599

Reaction: Central Ring Cleavage

Structure: Transition state
Method: M06/6-31+G(2df,p)

7	0	8.854996	2.224920	2.221321
6	0	8.629763	1.580924	1.121955
6	0	8.402666	2.131023	-0.161828
8	0	8.644233	0.241079	1.273932
8	0	6.057535	0.985548	-0.461519
7	0	8.308799	2.625987	-1.208151
6	0	8.890955	0.130442	2.582228
6	0	6.098728	1.579551	-1.502318
7	0	9.032109	1.265157	3.186123
6	0	9.021878	-1.200675	3.190904
6	0	4.961409	1.562489	-2.636015
7	0	6.753431	2.369655	-2.276748
6	0	7.931117	-2.025317	3.463691
6	0	10.274179	-1.672838	3.580890
6	0	4.877737	0.531628	-3.573937
6	0	3.929835	2.499807	-2.631222
7	0	6.551202	-1.583119	3.143901
6	0	8.068079	-3.257952	4.075504
7	0	11.492593	-0.889784	3.275865
6	0	10.454220	-2.885229	4.218290
6	0	3.786566	0.388401	-4.410726
7	0	5.961346	-0.469791	-3.729558
6	0	2.827964	2.395240	-3.458788
7	0	3.964475	3.676664	-1.732358
8	0	5.683094	-2.421302	3.224191
8	0	6.399188	-0.420981	2.843239
1	0	7.200226	-3.877999	4.271155
6	0	9.335677	-3.663610	4.442180
8	0	11.484759	-0.244341	2.249829
8	0	12.406339	-0.984420	4.060492
1	0	11.441813	-3.217674	4.519341
1	0	3.741551	-0.425588	-5.125418
6	0	2.767547	1.316433	-4.319084
8	0	5.939124	-1.133451	-4.743655
8	0	6.774156	-0.561034	-2.839965
1	0	2.041885	3.141962	-3.437325
8	0	4.494292	3.539753	-0.655444
8	0	3.430187	4.680523	-2.150638
7	0	9.501816	-4.977386	5.103219
7	0	1.585886	1.166865	-5.193674
8	0	8.490087	-5.571314	5.400383
8	0	10.637117	-5.352349	5.293070
8	0	1.593543	0.239917	-5.973222
8	0	0.700068	1.982497	-5.061891

References:

[1] Klapötke, T.M.; Witkowski, T.G. 5,5'-Bis(2,4,6-trinitrophenyl)-2,2'-bi(1,3,4-oxadiazole) (TKX-55): Thermally Stable Explosive with Outstanding Properties. *ChemPlusChem* **2016**, *81*, 357 – 360.