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Supporting Information

Computational Details

Computations were carried out using the Gaussian 09 program suite.[1] The structure optimizations are performed with B3PW91 functional with 6-31G(d,p) basis set and characterized to be true local energy minima on the potential energy surface and no imaginary frequencies were found. The calculated total energies (E_0), zero point energies (ZPE), and thermal corrections (ΔH_T) at the B3PW91/6-31G(d,p) level for the peracid compounds are listed in Table S1. Isodesmic reactions were designed to compute the gas phase heats of formation (HOF_{Gas}) and summarized in Figure S2. The usage of the HOF_{Gas} in the calculation of detonation properties slightly overestimates the values of detonation velocity and detonation pressure, and hence, the solid phase HOF (HOF_{Solid}) have been calculated which can efficiently reduce the errors. The HOF_{Solid} is calculated as the difference between HOF_{Gas} and heat of sublimation (HOF_{Sub}) as,

$$HOF_{Solid} = HOF_{Gas} - HOF_{Sub} \quad (1)$$

The heat of sublimation (HOF_{Sub}), which is required to convert the HOF_{Gas} to the HOF_{Solid}, was calculated from Equation (2),[2]

$$HOF_{Sub} = 4.4307\ x\ 10^{-4}A^2 + 2.0599\left(v\sigma_{tot}^2\right)^{0.5} - 2.4825 \quad (2)$$

where A represent the surface area of the 0.001 electrons/bohr^3 isosurface of electronic density, *v* denotes the degree of balance between the positive and negative surface potentials, and σ_{tot}^2 is the electrostatic potential variance. These molecular surface properties were obtained using the Multiwfn program[3] and listed in Table S2.

The density has been referred to as "the primary physical parameter in detonation performance" of explosives.[4-10] For example, the important performance attribute of detonation velocity is proportional to density, while the detonation pressure is proportional to the square of the initial density.[11] An increase in density is also desirable in terms of the amount of material that can be packed into volume-limited warhead or propulsion configurations. The densities (ρ) for peracid compounds were calculated using the equation (3), as suggested by Politzer et al.[12] for CHNO energetic compounds,

$$\rho = 0.9183\left(\frac{M}{V_m}\right) + 0.0028\left(v\sigma_{tot}^2\right) + 0.0443 \quad (3)$$

where, M is the molecular mass in g/mol. V_m is the volume enclosed by the 0.001 au contour of the molecule's electronic density and $v\sigma_{tot}^2$ is an electrostatic interaction index.

Oxygen balance (OB) is one of the parameter of quantifying how well an explosive provides its own oxidant.[13] Most of the energy released comes from oxidation (reaction with oxygen), the amount of oxygen available is a critical factor. If excess oxygen molecules are remaining after the oxidation reaction, the oxidizer is said to have a 'positive' OB. If the oxygen molecules are completely consumed and excess fuel molecules remain, the oxidizer is said to have a 'negative' OB. If neutral OB (OB = 0%), means that there is exactly enough oxygen for the complete oxidation. It is reported that the heat of detonation (Q) reaches a maximum for an OB of zero, since this corresponds to the stoichiometric oxidation of carbon to carbon dioxide and hydrogen to water. The OB can therefore be used to optimize the composition of the explosive to give an OB as close to zero as possible. In addition, knowledge of OB in explosives can be applied is in the processing of mixtures of explosives. OB (%) for an explosive containing the general formula $C_aH_bN_cO_d$ with molecular mass M can be calculated as,

$$\mathrm{OB}(\%) = \frac{(d - 2a - 0.5b)}{M} \mathrm{X}\, 1600 \quad (4)$$

The detonation velocity (D in km/s) and detonation pressure (P in GPa) are the performance parameters, computed using the empirical Kamlet−Jacobs equations:[11]

$$N = \frac{2c + 2d + b}{48a + 4b + 56c + 64d} \quad (5)$$

$$M = \frac{56c + 88d - 8b}{2c + 2d + b} \quad (6)$$

$$Q = \frac{28.9b + 47\left(d - \frac{b}{2}\right) + HOF_{Explosive}}{12a + b + 14c + 16d} \quad (7)$$

$$D = 1.01(NM^{0.5}Q^{0.5})^{0.5}(1+1.30\rho) \quad (8)$$

$$P = 1.55\rho^2 NM^{0.5}Q^{0.5} \quad (9)$$

in which, N represents the moles of detonation gases per gram explosive, M is the average molecular weight of these gases(g/mol), Q denotes the heat of detonation (cal/g), and ρ is the predicted density of salts (g/cm^3).

The methodology proposed by Akhavan[14] has been used to predict explosive power and power index using the heat of detonation (Q) and volume (V) of gaseous explosion products. Power index is a comparative numerical value used to rank the relative power of an explosive based on the heat and volume of gases produced by detonation of 1.0 gram of explosive.

$$\text{Explosive Power} = Q\mathrm{V} \quad (10)$$

$$\text{Power Index} = \frac{Q\text{V}}{Q_{Picric\ acid}V_{\text{(Picric acid)}}}\text{x } 100 \quad (11)$$

In the present work, decomposition products of peracids are predicted by using the 'Kistiakowsky-Wilson' rules (K-W rules). These rules should only be used for moderately oxygen deficient explosives with an oxygen balance greater than – 40 %. Under these circumstances, the modified Kistiakowsky-Wilson rules are employed. The predicted decomposition reactions for the peracid compounds are summarized in Tables S3.

Kistiakowsky-Wilson Rules

1. Carbon atoms are converted to carbon monoxide.
2. If any oxygen remains then hydrogen is then oxidized to water.
3. If any oxygen still remains then carbon monoxide is oxidized to carbon dioxide.
4. All the nitrogen is converted to nitrogen gas, N_2.

Modified Kistiakowsky-Wilson Rules

1. Hydrogen atoms are converted to water.
2. If any oxygen remains then carbon is converted to carbon monoxide.
3. If any oxygen still remains then carbon monoxide is oxidized to carbon dioxide.
4. All the nitrogen is converted to nitrogen gas, N_2.

Brisance for $C_aH_bN_cO_d$ based explosives relative to TNT is calculated using the correlation suggested by Keshavarz et al[15] and given as following:

$$Bris_{rel/TNT} = 85.5 + 4.812c + 2.556\left(d - a - \frac{b}{2}\right) - 35.96Bris^{-} + 19.69Bris^{+} \quad (12)$$

Where in above equation, $Bris_{core}$ is the core brisance, which is based on the number of nitrogen atoms and the distribution of oxygen atoms between carbon and hydrogen atoms;

$Bris^{+}$ and $Bris^{-}$ are correcting positive and negative functions for those values obtained on the basis of $Bris_{core}$.

Gurney[16] developed a simple model that permits the estimation of the velocity of metal driven by a detonating explosive. This model assumes that a given explosive liberates a fixed amount of specific energy (E) on detonation that is converted to kinetic energy partitioned between the driven metal and gaseous products. The specific energy determines the amount of mechanical work for the acceleration of the surrounding metal that can be done by the explosive. The Gurney velocity ($\sqrt{2E}$) provides a more relevant absolute indicator of the ability of an explosive to accelerate material under a wide variety of initial densities and geometries of interest. The Gurney velocity is predicted using Kamlet and Finger (K-F) method,[17] equation (13) and validated with Hardesty and Kennedy (H-K) method,[18] equation (14).

$$\sqrt{\Delta E} = 0.887\emptyset^{0.5}\rho^{0.4} \quad (13)$$

$$\sqrt{\Delta E} = 0.6 + 0.54\sqrt{1.44\emptyset\rho} \quad (14)$$

Where in above equations, ρ is the density in g/cm^3 and Φ is the quantity used by Kamlet and Jacobs[11] to calculate detonation properties, depends on: 1. the number of moles of gaseous detonation products per gram of explosive, 2. the average molecular weight of these gases, and 3. the heat of detonation in calories per gram.

Most of the explosives contain C, H, N, and O atoms. During an explosive reaction, the molecule uses the oxygen atoms available within it and does not depend on the external, atmospheric oxygen; it probably has no time for that because of the fast nature of the explosive process. It must be noted that all oxidation reactions are exothermic.[19] The heat of combustion (ΔH_c) is defined as the heat evolved when 1 mole of a compound is completely burnt in excess of oxygen. It means that all C atoms and H atoms in the molecule are

converted into carbon dioxide (CO_2) and water (H_2O) combustion products, respectively. A fuel burning in air gives out heat of combustion. Heat of combustion is often referred to as the "calorific value." The HOFs of CO_2 and H_2O are -94.05 and -67.42 kcal/mol, respectively.

$$\Delta H_c = HOF_{combustion\ products} - HOF_{explosive} \quad (15)$$

List of Tables

Table S1. Total energy (E_0), zero point energy (ZPE), and thermal correction (ΔH_T) at the B3PW91/6-31G(d,p) Level for the peracid compounds.

Compd.	E_0 (a.u.)	ZPE (a.u.)	H_T (a.u.)
P1	-505.670443	0.0786	0.0083
P2	-710.071345	0.0809	0.0108
P3	-446.505225	0.0631	0.0068
P4	-650.904844	0.0654	0.0094
P5	-521.673247	0.0655	0.0083
P6	-462.505261	0.0500	0.0067
P7	-1070.874778	0.1184	0.0173
P8	-1011.712724	0.1029	0.0159
P9	-952.54976	0.0873	0.0145
P10	-893.385905	0.0718	0.0131
P11	-823.271299	0.0868	0.0133
P12	-764.106518	0.0713	0.0118
P13	-704.940844	0.0557	0.0103
P14	-1119.542072	0.1462	0.0180
P15	-1060.385217	0.1308	0.0164
P16	-1001.228414	0.1154	0.0149
P17	-1151.483972	0.1186	0.0178
P18	-1092.310948	0.1029	0.0163
P19	-1033.137028	0.0871	0.0149
P20	-1722.838004	0.1903	0.0280
P21	-1663.676906	0.1748	0.0275
P22	-1604.513721	0.1592	0.0251
P23	-1604.514394	0.1592	0.0251
P24	-1545.350456	0.1435	0.0237
P25	-1486.187057	0.1280	0.0223

P26	-1227.629657	0.1270	0.0197
P27	-1168.465153	0.1116	0.0182
P28	-1109.299896	0.0961	0.0167

Table S2. Molecular surface properties of peracid compounds.

Compd.	**Surface Area (Å^2)**	**Volume (Å^3)**	σ_{tot}^2 **(kJ/mol)**	ν
P1	141.1	127.3	1633.9	0.1819
P2	169.9	156.8	1153.5	0.1441
P3	126.0	111.6	1779.9	0.1680
P4	154.7	141.2	1362.7	0.1228
P5	137.0	122.8	1420.9	0.1739
P6	121.7	107.1	1521.3	0.1185
P7	239.3	231.1	715.9	0.1818
P8	225.4	215.9	766.9	0.1338
P9	211.4	200.7	841.0	0.0847
P10	201.3	185.4	927.2	0.0738
P11	191.9	181.7	728.9	0.1564
P12	177.9	166.4	786.2	0.1024
P13	163.8	151.2	883.7	0.0604
P14	269.4	262.1	1030.9	0.1697
P15	254.3	246.7	1138.5	0.1600
P16	239.2	231.3	1228.8	0.1364
P17	258.1	253.8	714.6	0.1546
P18	243.3	238.9	728.4	0.1296
P19	229.0	223.2	771.9	0.0968
P20	380.4	380.3	646.4	0.1800
P21	366.5	364.9	692.5	0.1641
P22	352.1	349.6	730.1	0.1332
P23	352.5	349.7	728.4	0.1271
P24	338.4	334.5	789.1	0.0994
P25	324.1	319.2	860.6	0.0713
P26	285.3	281.1	667.3	0.1570
P27	271.1	265.8	709.6	0.1246

P28	257.0	250.5	771.1	0.0923

Surface area and volume are computed on the 0.001 au molecular surfaces. σ_{tot}^{2} indicate the variability of the electrostatic potential, *v* is the degree of balance between the positive and the negative potentials on a molecular surface and is unitless.

Table S3. Decomposition reactions designed for the calculation of heat of detonation (Q).

Compd.	Decomposition reaction
P1	$C_3H_3N_3O_3 \rightarrow 1.5CO + 1.5H_2O + 1.5C + 1.5N_2$
P2	$C_3H_2N_4O_5 \rightarrow 2CO + CO_2 + H_2O + 2.5N_2$
P3	$C_2H_2N_4O_2 \rightarrow CO + H_2O + C + 2N_2$
P4	$C_2HN_5O_4 \rightarrow 0.5CO + 1.5CO_2 + 0.5H_2O + 2.5N_2$
P5	$C_2H_2N_4O_3 \rightarrow 2CO + H_2O + 2N_2$
P6	$CHN_5O_2 \rightarrow 0.5CO + 0.5CO_2 + 0.5H_2O + 2.5N_2$
P7	$C_6H_3N_3O_9 \rightarrow 4.5CO + 1.5CO_2 + 1.5H_2O + 1.5N_2$
P8	$C_5H_2N_4O_8 \rightarrow 3CO + 2CO_2 + H_2O + 2N_2$
P9	$C_4HN_5O_7 \rightarrow 1.5CO + 2.5CO_2 + 0.5H_2O + 2.5N_2$
P10	$C_3N_6O_6 \rightarrow 3CO_2 + 3N_2$
P11	$C_4H_2N_4O_6 \rightarrow 3CO + CO_2 + H_2O + 2N_2$
P12	$C_3HN_5O_5 \rightarrow 1.5CO + 1.5CO_2 + 0.5H_2O + 2.5N_2$
P13	$C_2N_6O_4 \rightarrow 2CO_2 + 3N_2$
P14	$C_6H_4N_8O_6 \rightarrow 4CO + 2H_2O + 2C + 4N_2$
P15	$C_5H_3N_9O_5 \rightarrow 3.5CO + 1.5H_2O + 4.5N_2 + 1.5C$
P16	$C_4H_2N_{10}O_4 \rightarrow 3CO + H_2O + 5N_2 + C$
P17	$C_4H_2N_{10}O_6 \rightarrow 3CO + CO_2 + H_2O + 5N_2$
P18	$C_3HN_{11}O_5 \rightarrow 1.5CO + 1.5CO_2 + 0.5H_2O + 5.5N_2$
P19	$C_2N_{12}O_4 \rightarrow 2CO_2 + 6N_2$
P20	$C_{10}H_4N_8O_{12} \rightarrow 10CO + 2H_2O + 4N_2$
P21	$C_9H_3N_9O_{11} \rightarrow 8.5CO + 0.5CO_2 + 1.5H_2O + 4.5N_2$
P22	$C_8H_2N_{10}O_{10} \rightarrow 7CO + CO_2 + H_2O + 5N_2$
P23	$C_8H_2N_{10}O_{10} \rightarrow 7CO + CO_2 + H_2O + 5N_2$
P24	$C_7HN_{11}O_9 \rightarrow 5.5CO + 1.5CO_2 + 0.5H_2O + 5.5N_2$
P25	$C_6N_{12}O_8 \rightarrow 4CO + 2CO_2 + 6N_2$
P26	$C_6H_2N_{10}O_6 \rightarrow 5CO + H_2O + 5N_2 + C$

P27	$C_5HN_{11}O_5 \rightarrow 4.5CO + 0.5H_2O + 5.5N_2 + 0.5C$
P28	$C_4N_{12}O_4 \rightarrow 4CO + 6N_2$

Table S4. Decomposition reactions designed for the calculation of heat of combustion (ΔH_c)

Compd.	Decomposition reaction
P1	$C_3H_3N_3O_3 + 2.25O_2 \rightarrow 3CO_2 + 1.5H_2O + 1.5N_2$
P2	$C_3H_2N_4O_5 + O_2 \rightarrow 3CO_2 + H_2O + 2.5N_2$
P3	$C_2H_2N_4O_2 + 1.5O_2 \rightarrow 2CO_2 + H_2O + 2N_2$
P4	$C_2HN_5O_4 + 0.25O_2 \rightarrow 2CO_2 + 0.5H_2O + 2.5N_2$
P5	$C_2H_2N_4O_3 + O_2 \rightarrow 2CO_2 + H_2O + 2N_2$
P6	$CHN_5O_2 + 0.25O_2 \rightarrow CO_2 + 0.5H_2O + 2.5N_2$
P7	$C_6H_3N_3O_9 + 2.25O_2 \rightarrow 6CO_2 + 1.5H_2O + 4.5N_2$
P8	$C_5H_2N_4O_8 + 1.5O_2 \rightarrow 5CO_2 + H_2O + 2N_2$
P9	$C_4HN_5O_7 + 0.75O_2 \rightarrow 4CO_2 + 0.5H_2O + 2.5N_2$
P10	$C_3N_6O_6 \rightarrow 3CO_2 + 3N_2$
P11	$C_4H_2N_4O_6 + 1.5O_2 \rightarrow 4CO_2 + H_2O + 2N_2$
P12	$C_3HN_5O_5 + 0.75O_2 \rightarrow 3CO_2 + 0.5H_2O + 2.5N_2$
P13	$C_2N_6O_4 \rightarrow 2CO_2 + 3N_2$
P14	$C_6H_4N_8O_6 + 4O_2 \rightarrow 6CO_2 + 2H_2O + 5N_2$
P15	$C_5H_3N_9O_5 + 3.25O_2 \rightarrow 5CO_2 + 1.5H_2O + 4.5N_2$
P16	$C_4H_2N_{10}O_4 + 2.5O_2 \rightarrow 4CO_2 + H_2O + 5N_2$
P17	$C_4H_2N_{10}O_6 + 1.5O_2 \rightarrow 4CO_2 + H_2O + 5N_2$
P18	$C_3HN_{11}O_5 + 0.75O_2 \rightarrow 3CO_2 + 0.5H_2O + 5.5N_2$
P19	$C_2N_{12}O_4 \rightarrow 2CO_2 + 6N_2$
P20	$C_{10}H_4N_8O_{12} + 5O_2 \rightarrow 10CO_2 + 2H_2O + 4N_2$
P21	$C_9H_3N_9O_{11} + 4.25O_2 \rightarrow 9CO_2 + 1.5H_2O + 4.5N_2$
P22	$C_8H_2N_{10}O_{10} + 3.5O_2 \rightarrow 8CO_2 + H_2O + 5N_2$
P23	$C_8H_2N_{10}O_{10} + 3.5O_2 \rightarrow 8CO_2 + H_2O + 5N_2$
P24	$C_7HN_{11}O_9 + 2.75O_2 \rightarrow 7CO_2 + 0.5H_2O + 5.5N_2$
P25	$C_6N_{12}O_8 + 2O_2 \rightarrow 6CO_2 + 6N_2$

P26	$C_6H_2N_{10}O_6 + 3.5O_2 \rightarrow \quad 6CO_2 + H_2O + 5N_2$
P27	$C_5HN_{11}O_5 + 2.75O_2 \rightarrow \quad 5CO_2 + 0.5H_2O + 5.5N_2$
P28	$C_4N_{12}O_4 + 2O_2 \rightarrow \quad 4CO_2 + 6N_2$

Table S5. Reported heat of formation in solid phase (HOF_{Solid}, kJ/mol), density (g/cm^3), detonation velocity (*D*, km/s), detonation pressure (*P*, GPa), chemical energy of detonation (*Q*, cal/g), explosive power (EP, kJ.dm^3/g^{-2}), and power index (PI, %) for TNT (2,4,6-trinitrotoluene) and RDX (hexahydro-1,3,5-trinitro-1,3,5-triazine).

Compd.	**HOF_{Solid} (kJ/mol)**	**Density (g/cm^3)**	***D*** **(km/s)**	***P*** **(GPa)**	**EP (kJ dm^3/g^{-2})**	**PI (%)**
TNT	-67.36[20]	1.64[21]	6.94[21]	22.0[21]	3143[14]	116[14]
RDX	79.08[20]	1.80[22]	8.60[22]	33.9[22]	4573[14]	169[14]

Table S6. Reported heat of combustion (ΔH_c, cal/g), brisance, and Gurney velocity ($\sqrt{2E}$, km/s) for TNT and RDX.

Compd.	**ΔH_c (cal/g)**	**Brisance**	**$\sqrt{2E}$ (km/s)**	
			K-F method	**H-K method**
TNT	3571	100[15]	2.37[17] (2.37)[17]	2.42[18]
RDX	2255[15]	140[15]	2.90[17] (2.93)[17]	2.85[18]

K-F method: Kamlet-Finger method [Ref. 17], H-K method: Hardesty- Kennedy method [Ref. 18]. The parenthesis values indicate the experimental data of Gurney velocity.

Table S7. Total energy (E_0) at 298K and HOF_{Gas} for the reference compounds used in isodesmic reactions at the B3PW91/6-31G(d,p) level.

Compd.	**E_0 (a.u.)**	**ZPE (a.u.)**	**H_T (a.u.)**	**HOF_{Gas} (kJ/mol)**
1,2,4-Triazole	-242.100673	0.060396	0.004479	192.7[23]

Tetrazole	-258.107670	0.047452	0.00439	320[24]
1,3,5-Triazine	-280.187731	0.065657	0.005073	225.8[25]
1,2,4,5-Tetrazine	-296.149971	0.051685	0.005188	487.2[a]
CH_3NNCH_3	-189.119052	0.084721	0.006074	159.44[a]
NH_2NNNH_2	-221.183657	0.063655	0.005455	307.49[a]
CH_3COOOH	-304.019595	0.064852	0.006847	-321.43[a]
CH_3NO_2	-244.866536	0.050348	0.005192	-81[26]
CH_4	-40.459760	0.045119	0.003812	-74.6[27]
NH_3	-56.499062	0.034638	0.003808	-45.94[28]

[a]Heat of formation calculated by the G3 composite method.

Table S8. Total energies (E_0), zero point energies (ZPE), and thermal corrections (ΔH_T) at the B3LYP functional with 6-31G, 6-311G(d,p), and aug-cc-pVTZ basis set for **P1**, **P2**, **P5** and **P11** peracid compounds.

Compd.	**E_0 (a.u.)**	**ZPE (a.u.)**	**H_T (a.u.)**
	B3LYP/6-31G		
P1	-505.66450	0.0765	0.0084
P2	-710.056637	0.0776	0.0110
P5	-521.654308	0.0625	0.0085
P11	-823.261360	0.0821	0.0137
B3LYP/6-311G(d,p)			
P1	-505.993635	0.0777	0.0083
P2	-710.527518	0.0798	0.0109
P5	-522.006434	0.0646	0.0084
P11	-823.807394	0.0856	0.0116
B3LYP/aug-cc-pVTZ			
P1	-506.58523	0.0776	0.0083
P2	-710.618888	0.0797	0.0109
P5	-522.074566	0.0646	0.0083
P11	-823.912757	0.0858	0.0133

Cartesian coordinates (Å) of the individual compounds studied in the present work at the B3PW91/6-31G(d,p) level

Compound: P1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.528776	0.457866	0.000262
2	7	0	-1.352206	1.093707	0.000376
3	6	0	-0.499945	0.074076	-0.000022
4	6	0	-2.353578	-0.883735	-0.000198
5	7	0	-1.069008	-1.162973	-0.000411
6	6	0	0.954584	0.326288	-0.000116
7	8	0	1.491934	1.415776	-0.000514
8	8	0	1.653381	-0.824541	0.000368
9	8	0	3.050574	-0.548511	0.000173
10	1	0	-3.384920	0.992545	0.000472
11	1	0	-3.168827	-1.593868	-0.000384
12	1	0	3.030191	0.439559	0.000121

Compound: P2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.083212	1.337747	-0.000081
2	6	0	1.477981	0.048297	0.000016
3	7	0	0.457599	-0.767784	0.000132
4	7	0	-0.244321	1.397034	-0.000114
5	6	0	-0.582327	0.104262	0.000026
6	7	0	2.886140	-0.293960	0.000004
7	8	0	3.187275	-1.468604	0.000093
8	8	0	3.646504	0.672587	-0.000036
9	6	0	-1.986567	-0.366036	0.000061
10	8	0	-2.336142	-1.526003	-0.000247
11	8	0	-2.851273	0.662923	0.000128
12	8	0	-4.191915	0.183391	0.000134
13	1	0	1.664243	2.166225	-0.000175
14	1	0	-4.032781	-0.790976	-0.000592

Compound: P3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.742541	1.158399	-0.000388
2	6	0	-0.029874	0.013597	-0.000002
3	6	0	-1.978418	0.703608	-0.000281
4	7	0	-0.712665	-1.117373	0.000387
5	7	0	-1.967238	-0.649409	0.000305
6	7	0	1.429223	0.001283	0.000005
7	8	0	1.969459	-1.094078	-0.000545
8	8	0	1.983792	1.087655	0.000528
9	1	0	-2.882631	1.296260	-0.000398
10	1	0	-2.741078	-1.298407	0.000076

Compound: P4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.022874	-0.752274	-0.000166
2	6	0	-1.032638	0.137305	-0.000109
3	6	0	1.008628	0.053575	-0.000047
4	7	0	-0.701334	1.422985	0.000198
5	7	0	0.627465	1.346951	0.000297
6	7	0	2.413915	-0.306208	-0.000089
7	8	0	2.699099	-1.484150	-0.000194
8	8	0	3.182729	0.652726	0.000055
9	7	0	-2.436769	-0.271469	-0.000054
10	8	0	-3.261140	0.627430	-0.000544
11	8	0	-2.650162	-1.470416	0.000574
12	1	0	1.217033	2.170102	0.000490

Compound: P5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-1.418846	0.963396	0.000091
2	6	0	-0.503352	-0.023324	0.000089
3	7	0	-1.140592	-1.177658	-0.000191
4	7	0	-2.633942	0.417173	0.000120
5	7	0	-2.452015	-0.868419	-0.000183
6	6	0	0.935717	0.273840	0.000219
7	8	0	1.387291	1.404898	-0.000264
8	8	0	1.688696	-0.827518	0.000248
9	8	0	3.071446	-0.490356	-0.000065
10	1	0	-1.279945	1.964873	0.000266
11	1	0	3.024049	0.494403	-0.000329

Compound: P6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.059245	-0.689080	0.000161
2	7	0	-0.795318	-1.162744	-0.000235
3	7	0	-2.079394	0.610406	0.000252
4	6	0	-0.038821	-0.095853	-0.000031
5	7	0	-0.805544	1.003431	-0.000287
6	7	0	1.406026	-0.023080	-0.000047
7	8	0	1.860809	1.118541	0.000140
8	8	0	2.026097	-1.065226	0.000074
9	1	0	-0.527994	1.976072	-0.000432

Compound: P7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.861688	-1.065378	-0.000116
2	6	0	-0.463175	-1.203891	-0.000278
3	6	0	1.274211	0.200714	0.000268
4	7	0	-1.353356	-0.213565	-0.000321
5	7	0	0.491830	1.278878	0.000276
6	6	0	-0.810855	1.003037	-0.000113
7	6	0	2.758471	0.474668	0.000676
8	8	0	3.259870	1.575886	0.002403
9	8	0	3.466142	-0.661718	-0.001008
10	8	0	4.858749	-0.379036	-0.000463
11	6	0	-1.790180	2.151422	-0.000326
12	8	0	-2.994536	2.034870	-0.000406
13	8	0	-1.160027	3.332628	-0.000495
14	8	0	-2.101409	4.397081	-0.000487
15	6	0	-0.968064	-2.626177	-0.000684

16	8	0	-0.265151	-3.611041	-0.003081
17	8	0	-2.306062	-2.670568	0.002154
18	8	0	-2.757961	-4.017825	0.001835
19	1	0	4.846825	0.607831	0.001358
20	1	0	-2.949882	3.892920	-0.000451
21	1	0	-1.897436	-4.501155	-0.000645

Compound: P8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.306964	0.751753	0.034348
2	6	0	0.277604	1.576174	0.003442
3	6	0	0.942733	-0.532548	0.012388
4	7	0	-1.007778	1.284671	-0.019188
5	7	0	-0.309652	-0.983952	0.014379
6	6	0	-1.238471	-0.030058	0.013731
7	6	0	2.021155	-1.587527	-0.004898
8	8	0	1.822987	-2.779503	0.045556
9	8	0	3.238123	-1.037611	-0.088019
10	8	0	4.239744	-2.044567	-0.106679
11	6	0	-2.692043	-0.432692	0.051858
12	8	0	-3.618436	0.336659	0.165107
13	8	0	-2.833469	-1.758546	-0.056474
14	8	0	-4.207434	-2.117185	-0.018138
15	7	0	0.613381	3.030669	-0.007165
16	8	0	0.003081	3.709644	-0.810326
17	8	0	1.462528	3.384597	0.788118
18	1	0	3.686310	-2.859367	-0.047961
19	1	0	-4.629568	-1.230624	0.079048

Compound: P9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.554728	1.001262	0.024070
2	6	0	0.748189	1.201400	-0.007436
3	6	0	-0.889465	-0.290894	0.020414
4	7	0	1.713587	0.298679	-0.002951
5	7	0	-0.032504	-1.313446	0.003396
6	6	0	1.229231	-0.931685	0.011665
7	6	0	-2.351192	-0.661920	0.046018
8	8	0	-2.773769	-1.784193	0.199082

9	8	0	-3.126445	0.413547	-0.126959
10	8	0	-4.498641	0.049468	-0.104344
11	7	0	2.243886	-2.024833	0.035272
12	8	0	3.158426	-1.877818	0.822868
13	8	0	2.048464	-2.945016	-0.734200
14	7	0	1.192746	2.625323	-0.047550
15	8	0	2.088270	2.875799	-0.830771
16	8	0	0.612710	3.382466	0.705691
17	1	0	-4.433620	-0.924327	0.039446

Compound: P10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.208000	1.355700	-0.000192
2	6	0	1.179058	0.459088	0.000133
3	6	0	-0.987227	0.791566	-0.000010
4	7	0	1.070043	-0.858108	0.000512
5	7	0	-1.278095	-0.497728	-0.000024
6	6	0	-0.191921	-1.250787	0.000159
7	7	0	-2.150446	1.724652	0.000125
8	8	0	-3.052380	1.441034	-0.763169
9	8	0	-2.068968	2.666663	0.763360
10	7	0	2.568456	1.000148	-0.000058
11	8	0	2.774920	1.918922	-0.768030
12	8	0	3.342141	0.463103	0.767748
13	7	0	-0.418052	-2.724839	-0.000091
14	8	0	-1.277466	-3.125294	0.759892
15	8	0	0.281904	-3.364176	-0.760250

Compound: P11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.786451	-1.110425	-0.000704
2	7	0	-0.518415	-1.262996	-0.000709
3	6	0	1.254142	0.144098	-0.000173
4	6	0	-1.254142	-0.144098	-0.000171
5	7	0	0.518415	1.262996	0.000136
6	7	0	-0.786451	1.110425	0.000166
7	6	0	2.741850	0.352208	-0.000079
8	8	0	3.290029	1.430940	-0.000391
9	8	0	3.399936	-0.814203	0.000436
10	8	0	4.803808	-0.592494	0.000564
11	6	0	-2.741850	-0.352207	0.000072
12	8	0	-3.290028	-1.430940	0.000391

13	8	0	-3.399935	0.814203	-0.000085
14	8	0	-4.803809	0.592494	0.000253
15	1	0	4.835756	0.393793	0.000134
16	1	0	-4.835756	-0.393793	0.000402

Compound: P12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.119452	1.303518	0.169762
2	7	0	-1.192174	1.215087	0.124749
3	6	0	0.806424	0.161387	0.027633
4	6	0	-1.685351	-0.011146	-0.000885
5	7	0	0.284837	-1.061858	-0.130549
6	7	0	-1.027755	-1.157911	-0.115956
7	6	0	2.301896	0.303576	0.055823
8	8	0	2.892969	1.339939	0.254276
9	8	0	2.907675	-0.868352	-0.169546
10	8	0	4.319845	-0.713336	-0.139956
11	7	0	-3.162481	-0.111357	-0.015393
12	8	0	-3.640763	-0.986815	0.680893
13	8	0	-3.740918	0.692592	-0.721758
14	1	0	4.398577	0.252534	0.045006

Compound: P13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.658377	1.195840	0.026832
2	7	0	-0.658379	1.195781	-0.028238
3	6	0	1.235376	0.000063	-0.000333
4	6	0	-1.235310	0.000009	-0.000381
5	7	0	0.658405	-1.195770	-0.028305
6	7	0	-0.658266	-1.195799	0.027010
7	7	0	2.716854	0.000086	0.000277
8	8	0	3.244804	-0.759392	-0.789019
9	8	0	3.244012	0.759503	0.790212
10	7	0	-2.716925	-0.000112	0.000225
11	8	0	-3.243933	-0.759186	0.790543

12	8	0	-3.244989	0.758996	-0.789277

Compound: P14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.213999	-0.593568	-0.117241
2	7	0	0.213962	0.593546	-0.117217
3	6	0	1.592277	0.689340	-0.116190
4	7	0	2.149871	1.926149	-0.123604
5	7	0	2.557972	-0.219397	-0.102826
6	7	0	3.474364	1.855418	-0.128386
7	6	0	3.681633	0.534811	-0.107947
8	6	0	-1.592314	-0.689361	-0.116201
9	7	0	-2.149909	-1.926171	-0.123663
10	7	0	-2.558009	0.219375	-0.102783
11	7	0	-3.474402	-1.855442	-0.128414
12	6	0	-3.681668	-0.534835	-0.107927
13	6	0	-5.063640	0.019139	-0.220900
14	8	0	-5.266319	1.291957	0.219063
15	8	0	-5.961154	-0.559266	-0.770042
16	8	0	-4.330717	1.714993	1.225542
17	6	0	5.063606	-0.019151	-0.221005
18	8	0	5.266370	-1.291932	0.219031
19	8	0	5.961101	0.559302	-0.770126
20	8	0	4.330918	-1.714929	1.225666
21	1	0	1.674001	2.818657	-0.126376
22	1	0	-1.674038	-2.818679	-0.126479
23	1	0	-3.511955	1.831959	0.704747
24	1	0	3.512086	-1.831946	0.704993

Compound: P15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.015482	0.711291	0.048310
2	7	0	-0.498537	-0.440927	-0.121476
3	6	0	-1.881789	-0.468463	-0.108835
4	7	0	-2.497596	-1.667647	-0.286247
5	7	0	-2.794652	0.480767	0.049100
6	7	0	-3.817745	-1.532987	-0.249132
7	6	0	-3.928826	-0.222240	-0.045393
8	6	0	1.364830	0.749323	0.038242
9	7	0	1.971393	1.950105	0.213021
10	7	0	2.293237	-0.186532	-0.108141
11	7	0	3.291055	1.831183	0.173084
12	6	0	3.445846	0.516286	-0.016622
13	6	0	4.802910	-0.064574	-0.241124
14	8	0	4.959115	-1.398299	-0.014033
15	8	0	5.716515	0.559686	-0.707248
16	8	0	4.020186	-1.942175	0.929297
17	7	0	-5.248430	0.397873	0.066991
18	8	0	-5.267174	1.602733	0.249312
19	8	0	-6.209941	-0.347010	-0.031900
20	1	0	-2.069267	-2.572797	-0.432371
21	1	0	1.529351	2.848451	0.359093
22	1	0	3.189780	-1.939005	0.413688

Compound: P16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.269437	-0.569353	-0.000091

2	7	0	0.269439	0.569353	0.000128
3	6	0	1.651921	0.532961	-0.000085
4	7	0	2.317706	1.718304	-0.000052
5	7	0	2.523768	-0.466900	-0.000580
6	7	0	3.630278	1.524850	-0.000431
7	6	0	3.686386	0.194398	-0.000186
8	6	0	-1.651920	-0.532961	0.000124
9	7	0	-2.317705	-1.718304	0.000090
10	7	0	-2.523767	0.466899	0.000623
11	7	0	-3.630277	-1.524850	0.000475
12	6	0	-3.686385	-0.194398	0.000235
13	7	0	4.978748	-0.489866	0.000139
14	8	0	4.946631	-1.708225	-0.000233
15	8	0	5.970958	0.220466	0.000584
16	7	0	-4.978749	0.489866	-0.000061
17	8	0	-4.946638	1.708226	0.000154
18	8	0	-5.970959	-0.220465	-0.000784
19	1	0	1.925726	2.651653	0.000152
20	1	0	-1.925724	-2.651653	-0.000116

Compound: P17

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.958197	-1.369302	-0.039075
2	6	0	2.467571	-0.103338	0.096149
3	7	0	3.765140	-0.188943	-0.029051
4	7	0	2.986597	-2.224137	-0.259600
5	7	0	4.045336	-1.512324	-0.252111
6	6	0	1.697319	1.111402	0.519764
7	8	0	1.038613	1.166502	1.520520
8	8	0	1.885700	2.069258	-0.405399
9	8	0	1.299482	3.304111	0.004875
10	7	0	0.698897	-1.888722	-0.051983
11	7	0	-0.135277	-0.967876	-0.092839
12	7	0	-1.424430	-1.404867	-0.068756
13	7	0	-1.865523	-2.682608	-0.015719
14	7	0	-3.145431	-2.604080	0.051690
15	6	0	-2.503178	-0.573462	-0.009242
16	7	0	-3.580109	-1.313307	0.067265
17	6	0	-2.488681	0.908183	0.003845
18	8	0	-3.235668	1.612989	0.635275
19	8	0	-1.526649	1.390681	-0.811107
20	8	0	-1.499065	2.814661	-0.750679
21	1	0	0.367771	3.179863	-0.273694
22	1	0	-2.229041	2.990980	-0.106012

Compound: P18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.605297	-1.431905	-0.075515

2	6	0	2.377364	-0.302153	0.002164
3	7	0	3.617259	-0.659144	-0.220079
4	7	0	2.413821	-2.478520	-0.361441
5	7	0	3.597210	-2.003472	-0.450689
6	6	0	1.948315	1.041815	0.461612
7	8	0	1.150750	1.261529	1.347051
8	8	0	2.610582	1.986444	-0.206964
9	8	0	2.281768	3.281163	0.280599
10	7	0	0.271591	-1.707174	0.019098
11	7	0	-0.398331	-0.665994	-0.086686
12	7	0	-1.733924	-0.906159	0.056303
13	7	0	-2.316708	-2.061599	0.467497
14	7	0	-3.573682	-1.814591	0.535464
15	6	0	-2.718505	0.019387	-0.082151
16	7	0	-3.864099	-0.523578	0.202034
17	7	0	-2.523034	1.388705	-0.539426
18	8	0	-1.636007	1.554692	-1.362602
19	8	0	-3.273193	2.219518	-0.069412
20	1	0	1.617963	3.062964	0.974956

Compound: P19

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.170394	-2.025745	0.523449
2	7	0	1.892484	-2.093588	0.448986
3	7	0	3.640941	-0.784956	0.202043
4	7	0	1.479016	-0.862246	0.049563
5	6	0	2.584976	-0.081838	-0.075602
6	7	0	0.189685	-0.441106	-0.083338
7	7	0	-0.609391	-1.393348	-0.066425
8	7	0	-1.894607	-0.935196	-0.140950
9	7	0	-2.838427	-1.817912	-0.548602
10	6	0	-2.515890	0.264894	0.048373
11	7	0	-3.942460	-1.172625	-0.586784
12	7	0	-3.781975	0.130382	-0.210945
13	7	0	2.585354	1.303163	-0.529755
14	8	0	3.458470	2.012915	-0.075789
15	8	0	1.716557	1.596203	-1.336886
16	7	0	-1.925057	1.466222	0.625539
17	8	0	-1.225635	1.284535	1.610335
18	8	0	-2.221418	2.517639	0.100329

Compound: P20

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.487228	-1.335900	-0.176968
2	6	0	-3.793078	-1.111586	-0.049934
3	6	0	-1.756774	-0.225038	-0.182514
4	7	0	-4.382387	0.082091	0.012672
5	7	0	-2.208105	1.026166	-0.121648
6	6	0	-3.535273	1.108012	-0.039647
7	7	0	-0.357862	-0.442130	-0.361470
8	7	0	0.339588	0.249065	0.399388
9	6	0	1.738803	0.032415	0.219647
10	6	0	3.774638	0.925894	0.088436
11	7	0	2.468757	1.144760	0.224493
12	7	0	4.364377	-0.266568	0.012267
13	6	0	3.518417	-1.293796	0.062661
14	7	0	2.191198	-1.216665	0.148272
15	6	0	-4.167538	2.477312	0.012977
16	8	0	-5.334459	2.694340	0.247495
17	8	0	-3.271576	3.439417	-0.241307
18	8	0	-3.889397	4.718544	-0.193727
19	6	0	-4.659448	-2.345455	0.014299
20	8	0	-4.245643	-3.482197	0.046891
21	8	0	-5.960724	-2.030735	0.030805
22	8	0	-6.754540	-3.207967	0.091672
23	6	0	4.700868	2.115613	0.029522
24	8	0	5.905892	2.052793	-0.060039
25	8	0	4.021935	3.268550	0.085022
26	8	0	4.914325	4.373047	0.025010
27	6	0	4.083901	-2.692658	0.024150
28	8	0	3.441769	-3.704449	0.192489
29	8	0	5.399555	-2.683053	-0.223522

30	8	0	5.907784	-4.009948	-0.256066
31	1	0	-4.818425	4.466097	0.023724
32	1	0	-6.053156	-3.902319	0.101455
33	1	0	5.781122	3.905686	-0.041552
34	1	0	5.085630	-4.526206	-0.078033

Compound: P21

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.164197	-0.524247	0.171037
2	7	0	-0.494754	0.102659	-0.675921
3	6	0	-1.899864	-0.063764	-0.518716
4	7	0	-2.428671	0.055364	0.696960
5	7	0	-2.566720	-0.248716	-1.659024
6	6	0	-3.757730	-0.010032	0.714087
7	6	0	-3.870052	-0.306738	-1.474757
8	7	0	-4.547072	-0.180468	-0.349484
9	6	0	1.566425	-0.275755	0.073745
10	7	0	2.327491	-1.354878	0.224653
11	7	0	1.982847	0.980104	-0.072082
12	6	0	3.632403	-1.094521	0.176551
13	6	0	3.309161	1.104823	-0.059059
14	7	0	4.187722	0.110229	0.050525
15	6	0	3.901800	2.486760	-0.188865
16	8	0	5.082698	2.728786	-0.289863
17	8	0	2.950620	3.429419	-0.174983
18	8	0	3.530079	4.721662	-0.293872
19	6	0	4.537610	-2.296555	0.289713
20	8	0	4.160326	-3.445495	0.335706
21	8	0	5.826166	-1.937279	0.333760
22	8	0	6.657952	-3.084451	0.440247
23	6	0	-4.401304	0.133111	2.071280
24	8	0	-3.815836	0.437063	3.085254
25	8	0	-5.712951	-0.124977	2.018047
26	8	0	-6.299811	0.009593	3.304760
27	7	0	-4.688321	-0.530202	-2.705135
28	8	0	-5.701223	0.135873	-2.798531
29	8	0	-4.256063	-1.355682	-3.486957

30	1	0	4.487663	4.489806	-0.351920
31	1	0	5.981580	-3.803085	0.446318
32	1	0	-5.512622	0.264281	3.842478

Compound: P22

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.069659	-0.548482	-0.339458
2	7	0	0.793056	0.066227	0.462391
3	6	0	2.180358	-0.108714	0.212106
4	7	0	2.634498	0.043723	-1.033525
5	7	0	2.922264	-0.334849	1.296909
6	6	0	3.950912	0.016629	-1.101531
7	6	0	4.212582	-0.367263	1.035486
8	7	0	4.819601	-0.158477	-0.120992
9	6	0	-1.320219	-0.282444	-0.142355
10	7	0	-2.103894	-1.349460	-0.252036
11	7	0	-1.705950	0.976750	0.047804
12	6	0	-3.398821	-1.072387	-0.108934
13	6	0	-3.028235	1.119972	0.129287
14	7	0	-3.925885	0.138351	0.069516
15	6	0	-3.590138	2.508050	0.317576
16	8	0	-4.757996	2.764968	0.499190
17	8	0	-2.627044	3.436442	0.255839
18	8	0	-3.175988	4.735220	0.432568
19	6	0	-4.326631	-2.260917	-0.170210
20	8	0	-3.968933	-3.414396	-0.245713
21	8	0	-5.609611	-1.882681	-0.130143
22	8	0	-6.464119	-3.016374	-0.188013
23	7	0	4.537358	0.209060	-2.462744
24	8	0	5.517720	0.925177	-2.520813
25	8	0	3.970925	-0.369928	-3.369511
26	7	0	5.106036	-0.658705	2.197073
27	8	0	6.123754	0.002157	2.263276
28	8	0	4.719674	-1.527957	2.954647

29	1	0	-4.131653	4.518040	0.548795
30	1	0	-5.801458	-3.745578	-0.242506

Compound: P23

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.473115	0.006175	-0.439620
2	7	0	0.322679	-0.225985	0.485716
3	6	0	1.685911	-0.167317	0.075520
4	7	0	2.490600	0.480317	0.912143
5	7	0	2.045289	-0.814625	-1.034298
6	6	0	3.770782	0.459858	0.551618
7	6	0	3.351629	-0.800496	-1.218244
8	7	0	4.275990	-0.203157	-0.492757
9	6	0	-1.835399	-0.150303	-0.051411
10	7	0	-2.184555	-1.243192	0.628313
11	7	0	-2.651970	0.803261	-0.489226
12	6	0	-3.490439	-1.327896	0.799540
13	6	0	-3.930335	0.606168	-0.176195
14	7	0	-4.424657	-0.470249	0.440928
15	6	0	-4.940122	1.662240	-0.550985
16	8	0	-6.115961	1.624065	-0.270921
17	8	0	-4.369805	2.660447	-1.236046
18	8	0	-5.334873	3.646028	-1.575956
19	7	0	3.847085	-1.557617	-2.408555
20	8	0	3.188034	-1.442182	-3.424035
21	8	0	4.857154	-2.212501	-2.237490
22	7	0	-3.971771	-2.559245	1.497261
23	8	0	-4.965896	-3.079647	1.029176
24	8	0	-3.318105	-2.914603	2.459282
25	6	0	4.711236	1.246718	1.430343
26	8	0	4.376579	1.888430	2.399561
27	8	0	5.974177	1.151982	0.999727

28	8	0	6.843392	1.902829	1.835136
29	1	0	-6.149723	3.253344	-1.181545
30	1	0	6.203567	2.264272	2.493619

Compound: P24

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.273418	-0.917732	-0.478760
2	6	0	3.559183	-0.648904	-0.266088
3	6	0	1.451266	0.050999	-0.090440
4	7	0	4.045982	0.501455	0.208000
5	7	0	1.794974	1.218081	0.455720
6	6	0	3.103978	1.362240	0.538760
7	7	0	0.074582	-0.185436	-0.379691
8	7	0	-0.675564	0.120112	0.562211
9	6	0	-2.054948	-0.017551	0.242420
10	6	0	-3.814868	0.418114	-1.016608
11	7	0	-2.504477	0.509613	-0.897281
12	7	0	-4.672006	-0.169939	-0.200848
13	6	0	-4.068408	-0.670585	0.864499
14	7	0	-2.793162	-0.599932	1.187059
15	6	0	4.525942	-1.751622	-0.619934
16	8	0	4.207646	-2.837025	-1.048371
17	8	0	5.790956	-1.380657	-0.394465
18	8	0	6.686002	-2.431983	-0.726828
19	7	0	3.579216	2.670634	1.083472
20	8	0	4.534317	3.165112	0.516562
21	8	0	2.960180	3.105499	2.035525
22	7	0	-4.406858	1.052448	-2.233233
23	8	0	-3.787220	0.897448	-3.267379
24	8	0	-5.445455	1.659680	-2.058893
25	7	0	-4.950323	-1.392535	1.829514
26	8	0	-5.784179	-2.124839	1.332749

27	8	0	-4.740778	-1.175501	3.006748
28	1	0	6.054898	-3.125394	-1.033984

Compound: P25

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.212233	1.106485	0.050319
2	6	0	3.529367	1.157375	-0.006765
3	6	0	1.751494	-0.141912	0.134975
4	7	0	4.388879	0.153216	-0.009490
5	7	0	2.480621	-1.256504	0.102106
6	6	0	3.772807	-1.017027	0.004204
7	7	0	0.361412	-0.352519	0.361858
8	7	0	-0.361355	0.351971	-0.361996
9	6	0	-1.751451	0.141429	-0.134975
10	6	0	-3.772634	1.017024	-0.004904
11	7	0	-2.480415	1.256131	-0.103142
12	7	0	-4.388902	-0.153107	0.009737
13	6	0	-3.529533	-1.157400	0.007774
14	7	0	-2.212412	-1.106808	-0.049306
15	7	0	-4.125927	-2.523721	0.079162
16	8	0	-3.591044	-3.292795	0.854015
17	8	0	-5.081520	-2.722242	-0.645001
18	7	0	-4.653178	2.219293	0.082709
19	8	0	-4.266648	3.100762	0.825627
20	8	0	-5.661155	2.189179	-0.595162
21	7	0	4.653583	-2.219105	-0.084461
22	8	0	5.661702	-2.189240	0.593179
23	8	0	4.267073	-3.100139	-0.827903
24	7	0	4.125515	2.523914	-0.077423
25	8	0	3.588963	3.293945	-0.850123

26	8	0	5.082544	2.721576	0.645074

Compound: P26

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.178856	1.072590	0.293902
2	7	0	-3.478724	1.225058	0.215769
3	6	0	-1.721981	-0.189944	0.255179
4	6	0	-4.221340	0.113745	0.127527
5	7	0	-2.463582	-1.304983	0.266251
6	7	0	-3.764267	-1.143146	0.194626
7	7	0	-0.328249	-0.416446	0.329471
8	7	0	0.328238	0.416648	-0.329079
9	6	0	1.721969	0.190067	-0.254882
10	6	0	-5.697963	0.334338	-0.016473
11	8	0	-6.236594	1.417384	-0.058242
12	8	0	-6.361113	-0.826414	-0.105155
13	8	0	-7.755664	-0.591517	-0.248899
14	7	0	3.764300	1.143170	-0.194445
15	7	0	2.463611	1.305078	-0.265884
16	6	0	4.221333	-0.113746	-0.127556
17	7	0	3.478658	-1.225023	-0.215790
18	7	0	2.178793	-1.072482	-0.293742
19	6	0	5.697981	-0.334418	0.016076
20	8	0	6.236639	-1.417480	0.057031
21	8	0	6.361112	0.826288	0.105520
22	8	0	7.755683	0.591322	0.248967
23	1	0	-7.779070	0.395014	-0.236084
24	1	0	7.779106	-0.395199	0.235513

Compound: P27

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.724886	1.023007	-0.275026
2	7	0	3.025316	1.185246	-0.224683
3	6	0	1.275954	-0.238370	-0.178189
4	6	0	3.774169	0.081293	-0.101034
5	7	0	2.021334	-1.349518	-0.140762
6	7	0	3.322076	-1.179544	-0.095160
7	7	0	-0.117569	-0.471359	-0.236187
8	7	0	-0.773808	0.381250	0.396706
9	6	0	-2.170254	0.220160	0.235418
10	7	0	-4.190099	0.357266	1.232325
11	7	0	-2.887574	0.500136	1.331859
12	6	0	-4.647212	0.025415	0.029852
13	7	0	-3.958951	-0.160932	-1.089257
14	7	0	-2.650529	-0.085638	-0.979572
15	7	0	-6.115081	-0.131009	-0.078315
16	8	0	-6.647976	-0.742074	0.829448
17	8	0	-6.635009	0.363714	-1.060542
18	6	0	5.252785	0.313857	0.002315
19	8	0	5.786896	1.399473	-0.023493
20	8	0	5.921766	-0.838647	0.138020
21	8	0	7.317931	-0.593412	0.241472
22	1	0	7.338469	0.391107	0.177082

Compound: P28

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.449785	1.297179	0.585796
2	7	0	-3.753073	1.128432	0.588655
3	6	0	-1.722606	0.321022	0.026428
4	6	0	-4.198782	0.042621	-0.033908
5	7	0	-2.190434	-0.755477	-0.623215
6	7	0	-3.498109	-0.884096	-0.675474
7	7	0	-0.325758	0.546981	0.056150
8	7	0	0.326000	-0.505057	0.218196
9	6	0	1.721759	-0.299709	0.124090
10	7	0	3.755144	-0.946010	0.862251
11	7	0	2.449244	-1.068545	0.945908
12	6	0	4.199087	-0.051892	-0.013278
13	7	0	3.495881	0.686560	-0.863015
14	7	0	2.191205	0.538336	-0.813964
15	7	0	-5.667296	-0.141816	-0.031997
16	8	0	-6.164910	-0.479431	-1.089350
17	8	0	-6.221886	0.062578	1.031795
18	7	0	5.667537	0.127204	-0.069306
19	8	0	6.331735	-0.890712	-0.025201
20	8	0	6.054981	1.277804	-0.152230

Compound: 1,2,4-Triazole

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.865073	0.689544	-0.000013
2	7	0	-0.841222	-0.657933	0.000012
3	7	0	0.367308	1.159734	-0.000004
4	7	0	0.429903	-1.110139	0.000010
5	6	0	1.114595	0.022621	-0.000012
6	1	0	-1.777124	1.270566	-0.000015
7	1	0	-1.607724	-1.312560	0.000029
8	1	0	2.195792	0.027374	0.000002

Compound: 1H-Tetrazole

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.949072	-0.539660	0.000302
2	7	0	-0.704122	0.781569	-0.000085
3	7	0	0.203034	-1.171995	-0.000687
4	7	0	0.627474	0.973139	0.000104
5	7	0	1.153501	-0.203401	0.000403
6	1	0	-1.931270	-0.987063	0.000261
7	1	0	-1.333503	1.569844	-0.000217

Compound: 1,3,5-Triazine

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.286103	-0.115905	0.000004
2	7	0	0.577222	-1.246316	0.000002
3	6	0	-0.743429	-1.055804	0.000018
4	6	0	-0.542672	1.171706	-0.000036
5	7	0	0.790765	1.123036	-0.000001
6	1	0	-1.370150	-1.945904	0.000009
7	1	0	2.370325	-0.213615	0.000006
8	1	0	-1.000165	2.159507	0.000033
9	7	0	-1.367991	0.123284	0.000004

Compound: 1,2,4,5-Tetrazine

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.660133	1.193716	0.000007
2	7	0	-0.660133	1.193716	-0.000003
3	6	0	1.261922	-0.000001	0.000016
4	6	0	-1.261922	-0.000001	-0.000033
5	7	0	0.660135	-1.193716	0.000007
6	7	0	-0.660135	-1.193716	-0.000003
7	1	0	2.347913	0.000001	0.000002
8	1	0	-2.347913	0.000001	0.000042

Compound: $CH_3N{=}NCH_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.426056	0.451750	-0.000017
2	7	0	-0.426056	-0.451750	-0.000014
3	6	0	-1.789579	0.069354	0.000021
4	6	0	1.789579	-0.069354	-0.000007
5	1	0	-2.304719	-0.328814	-0.880891
6	1	0	-2.305000	-0.329579	0.880413
7	1	0	-1.820940	1.164293	0.000444
8	1	0	2.305095	0.329728	-0.880273
9	1	0	2.304624	0.328665	0.881031

10	1	0	1.820941	-1.164293	-0.000588

Compound: $H_2NN=NNH_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.435104	-0.446369	-0.011221
2	7	0	-0.435104	0.446376	0.011825
3	7	0	-1.707328	-0.067866	0.105566
4	7	0	1.707278	0.067818	-0.105972
5	1	0	-1.764228	-1.031990	-0.219129
6	1	0	-2.343935	0.542780	-0.389884
7	1	0	1.764366	1.032095	0.218221
8	1	0	2.344152	-0.542598	0.389409

Compound: $CH_3C(O)OOH$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.535942	1.370335	0.011595
2	6	0	-0.590923	-0.128372	0.003159
3	8	0	0.600779	-0.811659	-0.027726
4	8	0	-1.581605	-0.810222	0.010860
5	8	0	1.732052	0.085641	-0.068335
6	1	0	0.030202	1.732465	0.873040
7	1	0	-0.028917	1.742624	-0.882400
8	1	0	-1.559598	1.740907	0.045822
9	1	0	2.309695	-0.377851	0.556616

Compound: CH_3NO_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.318762	-0.004306	-0.002832
2	7	0	-0.173357	0.000026	-0.010696
3	8	0	-0.732425	-1.085988	0.002929
4	8	0	-0.723704	1.090529	0.002895
5	1	0	1.629734	0.032830	1.043327
6	1	0	1.658257	-0.927675	-0.468199
7	1	0	1.661970	0.884168	-0.529851

Compound: CH_4					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000003	-0.000003	0.000004
2	1	0	0.715278	0.350084	0.745724
3	1	0	-0.866418	-0.432945	0.502168
4	1	0	0.471432	-0.756563	-0.629007
5	1	0	-0.320275	0.839440	-0.618911

Compound: NH_3					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.118071
2	1	0	0.000000	0.936879	-0.275499
3	1	0	-0.811361	-0.468439	-0.275499
4	1	0	0.811361	-0.468439	-0.275499

List of Figures

Figure S1. Molecular structures of TATP and HMTD.

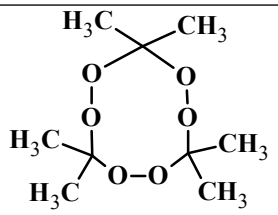
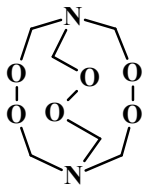
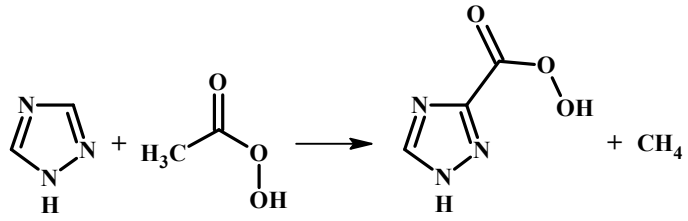
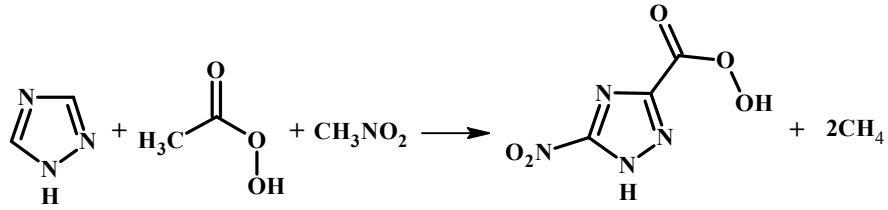
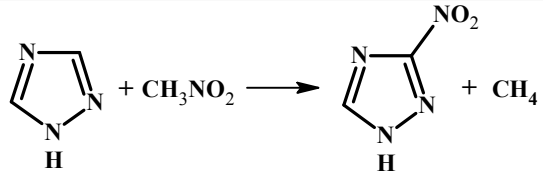
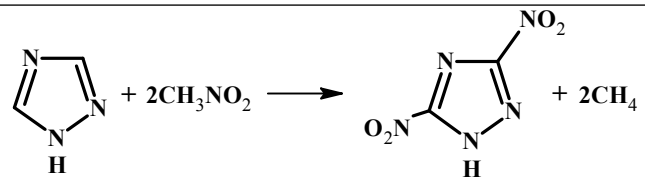
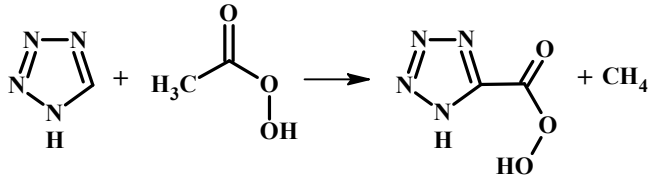
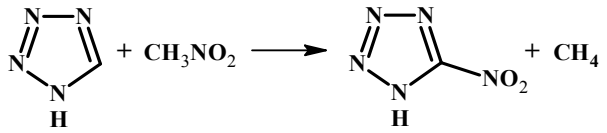
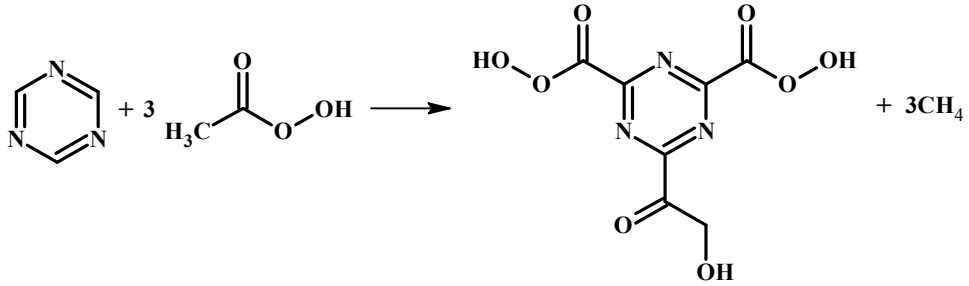
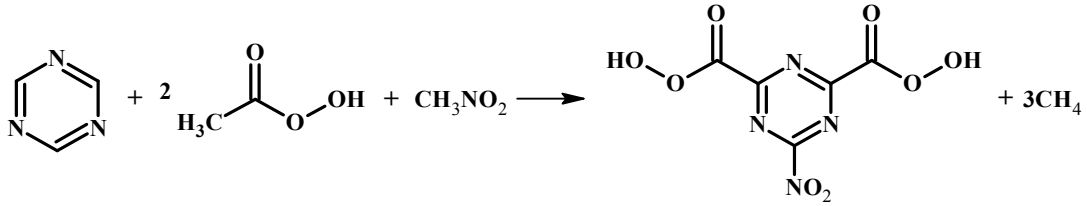
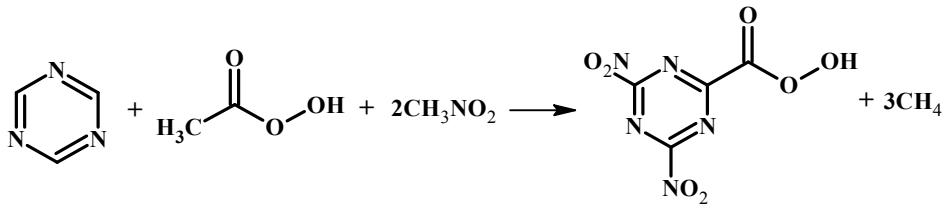
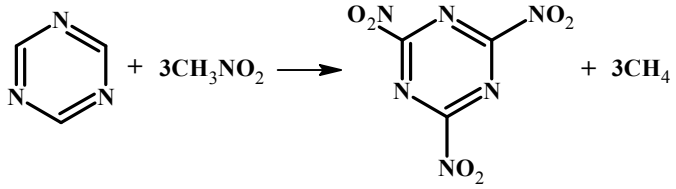
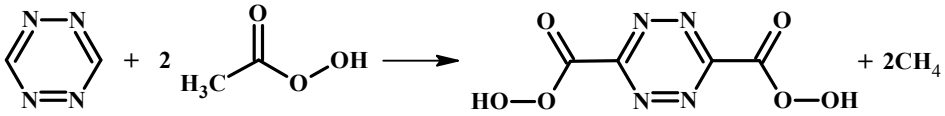
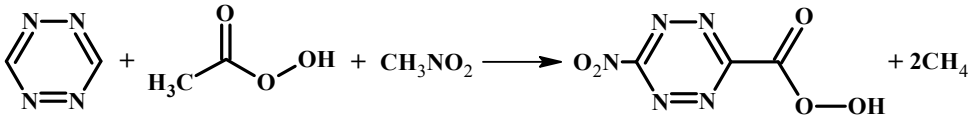
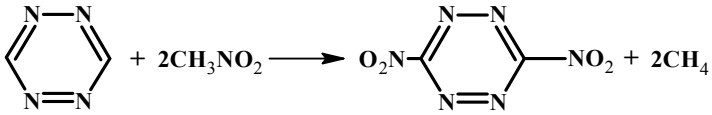
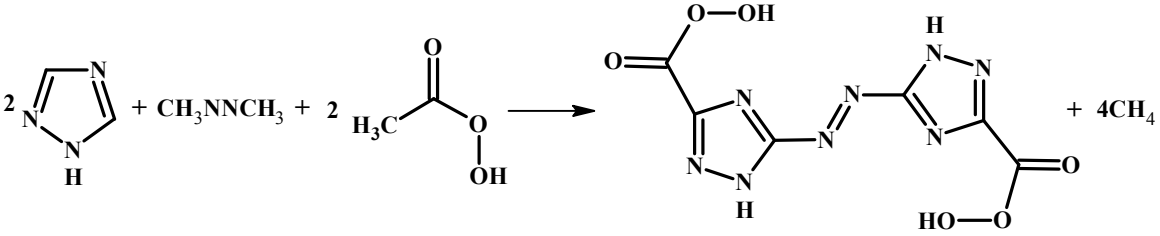
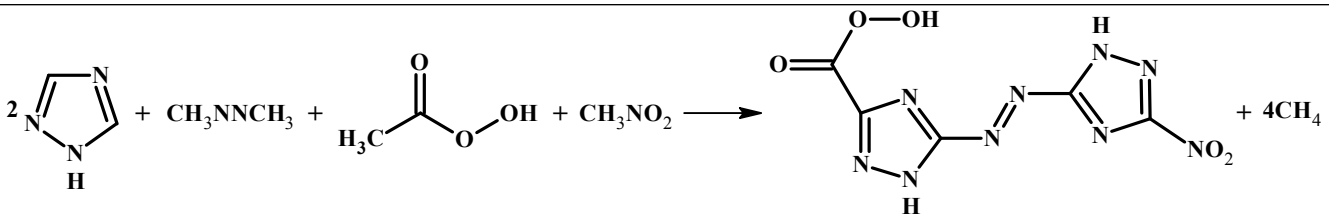
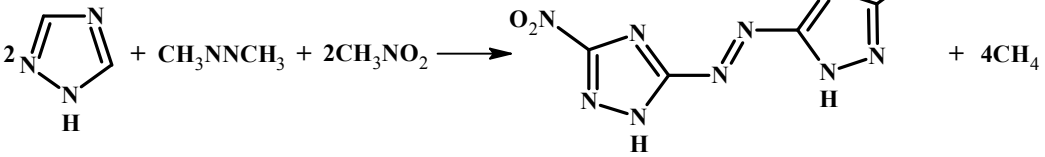
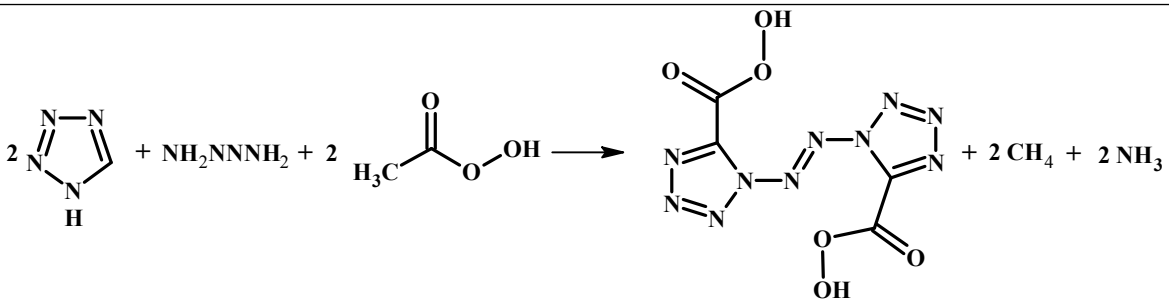
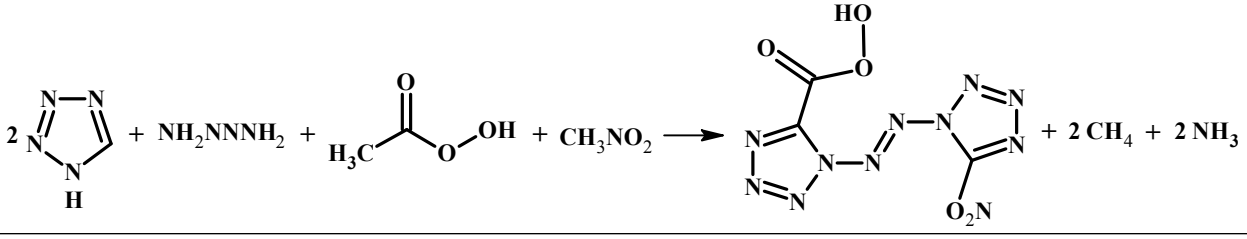
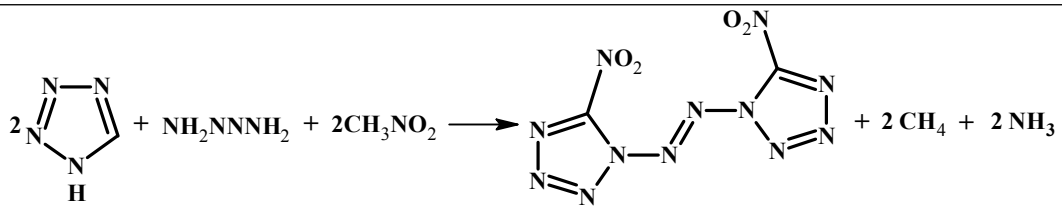
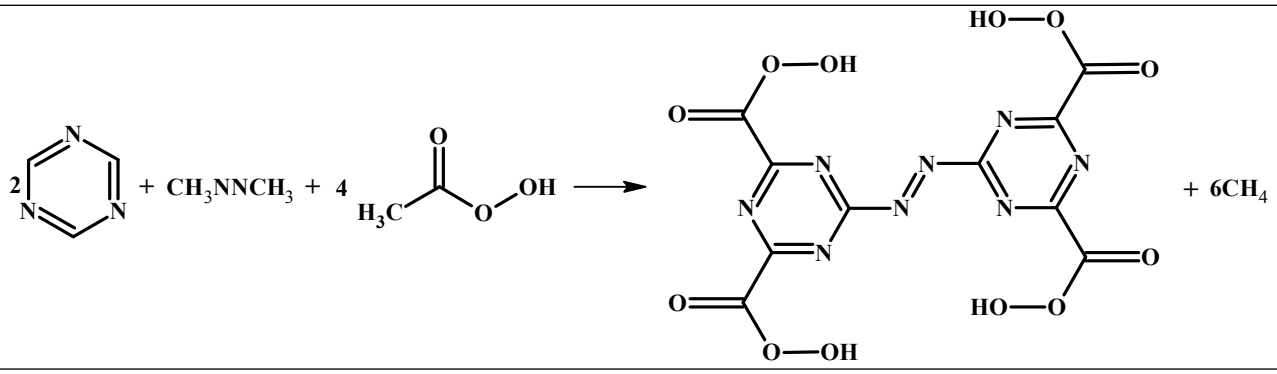
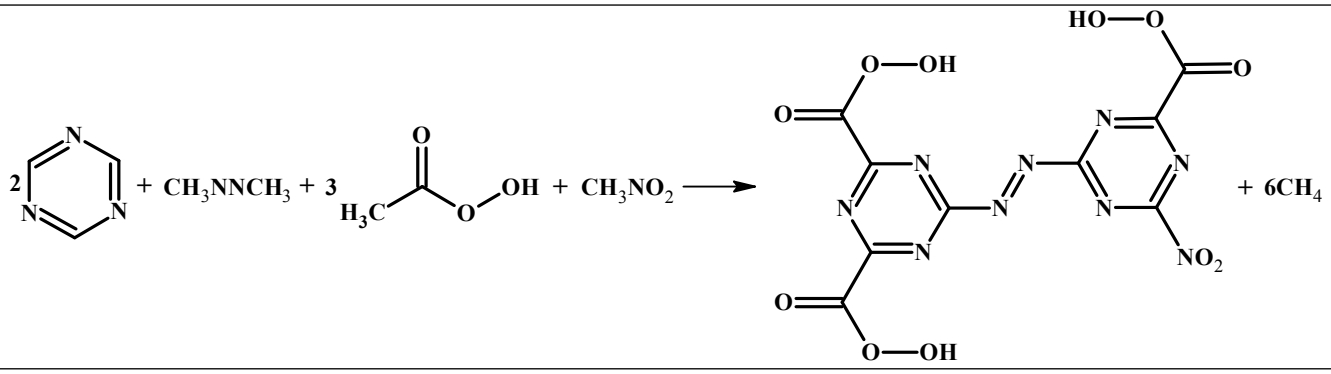
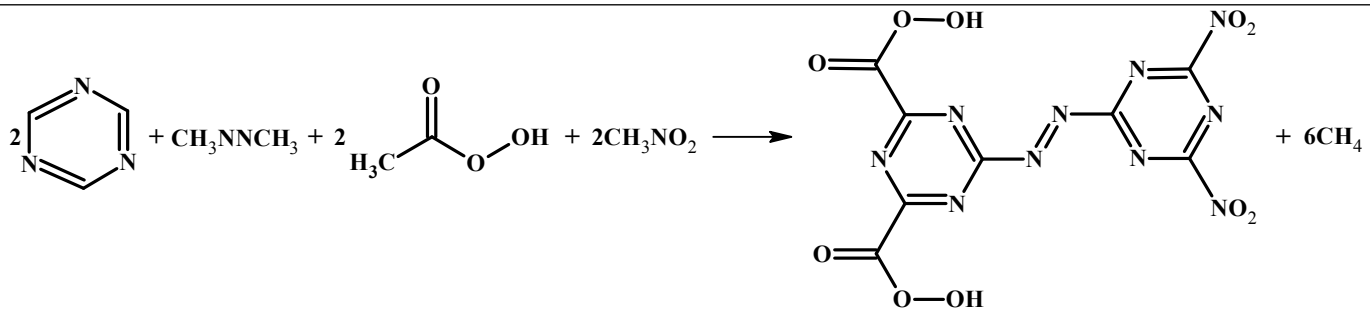
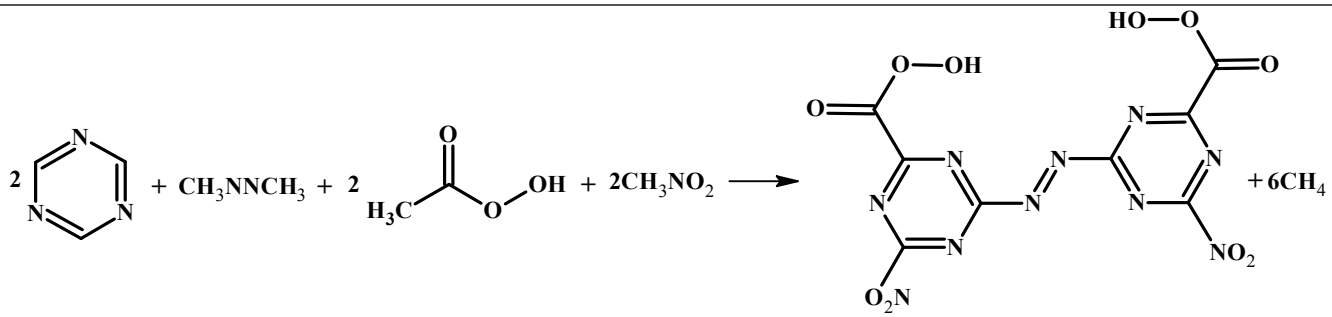
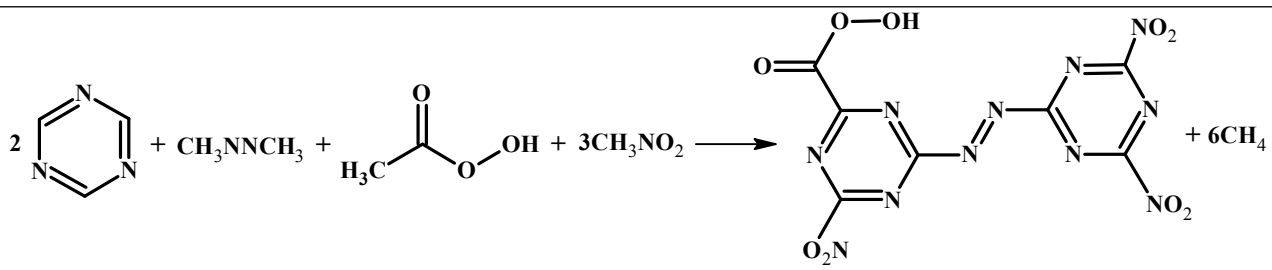
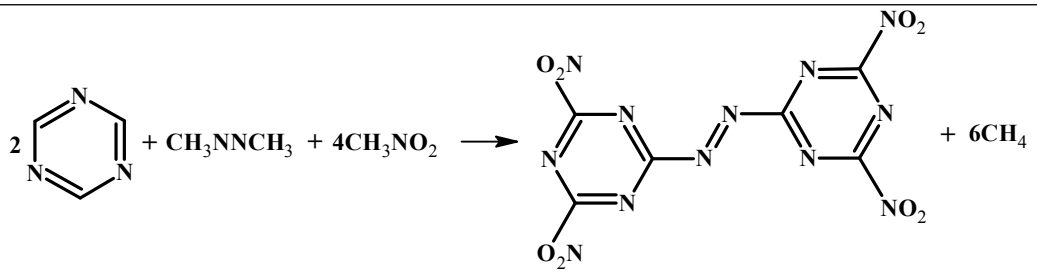
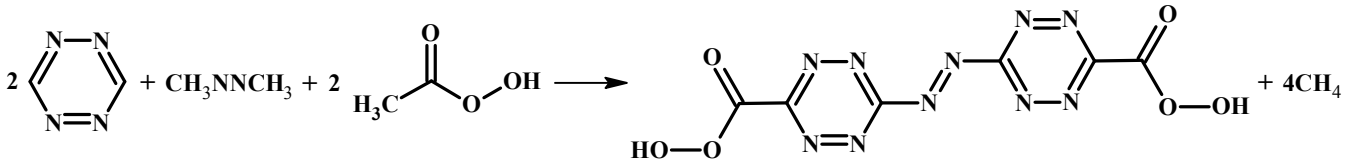
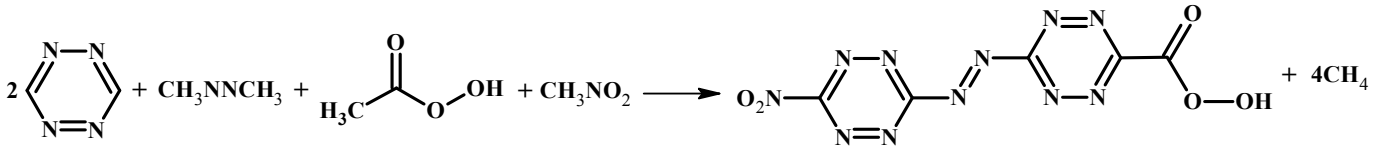
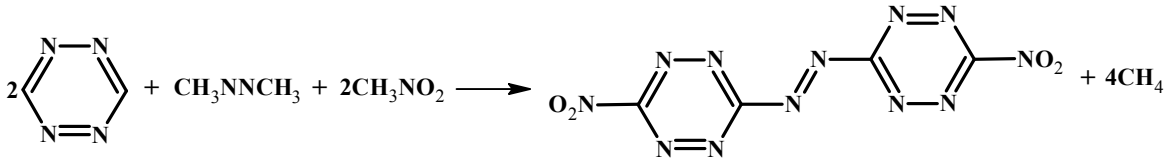
	
TATP (Triacetone triperoxide)	HMTD (Hexamethylene triperoxide diamine)

Figure S2. Designed isodesmic reactions for the prediction of gas phase HOF (HOF_{Gas}) of peracid compounds.

P1	
P2	
P3	
P4	
P5	
P6	
P7	
P8	
P9	

P10	
P11	
P12	
P13	
P14	
P15	
P16	
P17	
P18	

P19	
P20	
P21	
P22	
P23	
P24	

P25	
P26	
P27	
P28	

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