

Substituent Effects on the N–H Bond Dissociation Enthalpies, Ionization Energies, Acidities and Radical Scavenging Behavior of 3,7-Disubstituted-Phenoxazines and 3,7-Disubstituted-Phenothiazines

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Table S1. Modified Hammett, filed/inductive, resonance and excited electron constants of *para* substituents

Substituent (Y)	σ_p^+	σ_p^-	σ_F	σ_R	σ_p	$\sigma_{CC,p}^{ex}$
H	0.00	0.00	0.00	0.00	0.00	0.00
F	-0.07	-0.03	0.45	-0.39	0.06	-0.06
Cl	+0.11	+0.19	0.42	-0.19	0.23	0.22
CH ₃	-0.31	-0.17	0.01	-0.18	-0.17	-0.17
OCH ₃	-0.78	-0.26	0.29	-0.56	-0.27	-0.50
NH ₂	-1.30	-0.15	0.08	-0.74	-0.66	-0.88
CF ₃	+0.61	+0.65	0.38	0.16	0.54	-0.12
CN	+0.66	+1.00	0.51	0.15	0.66	-0.70
NO ₂	+0.79	+1.27	0.65	0.13	0.78	-1.17
(σ_p^+, σ_p^-) : Modified Hammett constant ¹ σ_F, σ_R : filed/inductive, resonance constant ¹ and $\sigma_p = \sigma_F + \sigma_R$ $\sigma_{CC,p}^{ex}$: excited electron constant ²						

Table S2. Selected analysis factors for assessing the fit of linear regression

Properties	System	R ²	RMSE ^a	F ^a	Prob(F) ^b
BDE (σ_p^+) ^d	PhozNH	0.9819	0.4028	379.6565	2.3400E-7
	PhtzNH	0.9831	0.3383	407.1609	1.8389E-7
IE (σ_p^+) ^d	PhozNH	0.9580	3.0297	159.81698	4.4786E-6
	PhtzNH	0.9465	3.0637	123.8979	1.0513E-5
PA (σ_p^-) ^e	PhozNH	0.9583	2.6832	168.2743	3.7637E-6
	PhtzNH	0.9601	2.6614	160.9298	4.37516E-6
BDE (σ_F, σ_R) ^f	PhozNH	0.9925	0.2754	230161.283	2.2205E-15
	PhtzNH	0.9824	0.3861	128282.405	1.2768E-14
IE (σ_F, σ_R) ^f	PhozNH	0.9925	2.0144	20014.0684	3.3664E-12
	PhtzNH	0.98147	1.9130	21819.5355	2.5980E-12
PA ($\sigma, \sigma_{CC,p}^{ex}$) ^f	PhozNH	0.97854	2.0863	77256.1184	5.8509E-14
	PhtzNH	0.97849	2.0280	82509.5329	4.8073E-14
Relative	PhozNH	0.9499	0.4724	132.8556	8.3278E-6

Energy of TS ^g	PhtzNH	0.9823	0.2594	388.2753	2.1659E-7
Relative	PhozNH	0.9513	0.8323	136.6716	7.5749E-6
Energy of PC ^g	PhtzNH	0.9915	0.3204	812.96751	1.67855E-8
^a RMSE: root mean squared error; ^b F: the ratio of the mean regression sum of squares divided by the mean error sum of squares. Prob(F): the probability that the null hypothesis for the full model is true					

Table S3. Calculated data for cross-validation

Test set	Linear Model	PhozNH	PhtzNH
		RMSE (kcal/mol)	
Cl, NH ₂ , NO ₂	BDE	0.41	0.15
	IE	3.76	3.48
	PA	3.91	3.81

Table S4. The relative enthalpies with respect to reactants of all species in PES of phenoxazine + HOO[•] and phenothiazine + HOO[•] in gas phase calculated at M05-2X-GD3/6-311++G(d,p)

Y	Phenoxazine + HOO [•]				Phenothiazine + HOO [•]			
	RC	TS	PC	P	RC	TS	PC	P
H	-8.1	0.6	-20.1	-9.9	-3.5	3.8	-16.3	-5.9
F	-4.7	0.0	-20.9	-11.3	4.0	3.1	-17.3	-7.3
Cl	-4.8	0.4	-19.9	-10.5	-4.1	3.7	-16.3	-6.4
CH ₃	-5.3	-0.3	-22.4	-11.3	-4.1	2.5	-18.3	-7.6
OCH ₃	-8.4	-1.8	-22.4	-13.6	-8.6	1.3	-20.5	-10.0
NH ₂	-8.7	-2.6	-27.0	-15.8	-8.8	0.2	-23	-11.5
CF ₃	-4.9	2.8	-16.1	-7.4	-5.4	5.5	-13.2	-4.0
CN	-4.8	3.3	-15.5	-6.9	-5.1	5.7	-13.0	-4.2
NO ₂	-5.5	3.9	-14.4	-6.2	-5.4	6.4	-11.7	-3.2

Table S5. The relative enthalpies with respect to reactants of all species in PES of PhozNH + HOO[•] and PhtzNHs + HOO[•] in benzene calculated at M05-2X-GD3/6-311++G(d,p)

Y	Phenoxazine + HOO [•]				Phenothiazine + HOO [•]			
	RC	TS	PC	P	RC	TS	PC	P
H	−5.3	3.2	−17.9	−9.2	−1.7	6.5	−13.8	−5.0
F	−5.1	2.8	−18.4	−10.2	−2.4	6.1	−14.5	−6.1
Cl	−5.3	3.4	−17.2	−9.2	−2.4	6.9	−13.3	−5.0
CH ₃	−3.3	2.1	−20.4	−10.8	−2.3	5.1	−16.0	−7.0
OCH ₃	−5.7	0.5	−22.2	−13.1	−5.6	3.9	−18.1	−9.4
NH ₂	−6.1	−0.5	−25.4	−15.7	−5.9	2.1	−21.1	−11.3
CF ₃	−2.8	5.9	−13.3	−5.9	−3.1	8.8	−10.2	−2.5
CN	−2.4	7.0	−12.2	−4.9	−5.4	9.3	−9.7	−2.4
NO ₂	−3.1	7.6	−11.0	−4.2	−2.9	10.2	−8.3	−1.3

Table S6. The radius of the reactants (RADn) and the reaction distance (RXD) (Å) in the HAT reactions with HOO[•] of PhozNH and PhtzNH compounds

Y	PhozNHs + HOO [•]			PhtzNHs + HOO [•]	
	RAD2	RAD1	RXD	RAD1	RXD
H	2.67	4.53	2.47	4.87	2.49
F		4.97	2.46	4.63	2.47
Cl		4.88	2.45	4.92	2.47
CH ₃		5.11	2.47	4.92	2.50
OCH ₃		5.02	2.49	5.35	2.51
NH ₂		4.85	2.47	4.74	2.53
CF ₃		4.93	2.43	5.07	2.45
CN		4.81	2.43	5.02	2.45
NO ₂		5.13	2.42	4.65	2.44
RAD1: calculated radius of PhozNH or PhtzNH; RAD2: radius of HOO [•] ; RXD: reaction distance in each reaction.					

Table S7. Dynamic viscosity (Pa.s) of benzene in liquid state at given temperatures³:

Benzene	
T (K)	Dynamic viscosity, Pa.s
298	6.04 E-04
303	5.91 E-04
323	4.36 E-04
348	3.35 E-04

Table S8. Data for linear correlation between $\log k$ of PhozNH + $\text{HOO}^\bullet$ and PhtzNH + $\text{HOO}^\bullet$ reactions in gas phase and benzene

Y	PhozNH			PhtzNH		
	$\log k$		$\frac{k_{\text{gas}}}{k_{\text{benzene}}}(\text{PhozNH})$	$\log k$		$\frac{k_{\text{gas}}}{k_{\text{benzene}}}(\text{PhtzNH})$
	Gas phase	Benzene		Gas phase	Benzene	
H	6.925828	5.934498	9.80233	5.636487896	3.73239376	80.1852
F	7.613842	5.146128	293.571	5.820857989	3.653212514	147.111
Cl	7.079181	4.944483	136.364	5.403120521	3.176091259	168.667
CH ₃	7.100371	5.380211	52.5	6.487138375	4.672097858	65.3191
OCH ₃	8.820858	7.113943	50.9231	6.750508395	4.792391689	90.8065
NH ₂	9.143015	7.230449	81.7647	7.773786445	4.892094603	761.538
CF ₃	5.858537	3.662758	156.957	5.862131379	3.544068044	208
CN	6.598791	4.113943	305.385	5.696356389	2.857332496	690.278
NO ₂	5.33646	2.80618	339.063	5.423245874	2.806179974	414.063

Table S9. Optimized Catersian Coordinates of all PhozNHs compounds

3,7-diY-PhozNH compounds				
Name of species: 3,7-di-H-PhozNH				Y=H, neutral
0 1				
C	3.52989200	-0.74519200	0.27252300	
C	2.32216000	-1.40414600	0.05921400	
C	1.17177000	-0.67335500	-0.15891300	
C	1.19482400	0.72214100	-0.15511500	
C	2.40050000	1.37299400	0.07258500	
C	3.56553100	0.64161100	0.27877000	
C	-1.19482500	0.72214100	-0.15511400	
C	-1.17177000	-0.67335400	-0.15891300	
C	-2.32216000	-1.40414600	0.05921300	
H	-2.25565100	-2.48282500	0.04878300	
C	-3.52989100	-0.74519200	0.27252200	
C	-3.56553100	0.64161000	0.27877000	
C	-2.40050100	1.37299500	0.07258700	
H	4.43245800	-1.31632300	0.43383700	
H	2.25565000	-2.48282500	0.04878500	
H	2.42397300	2.45528700	0.07602000	

H	4.49764400	1.16195600	0.44649900
H	0.00000100	2.38639200	-0.18717500
H	-4.43245800	-1.31632300	0.43383400
H	-4.49764500	1.16195500	0.44650000
H	-2.42397400	2.45528700	0.07602200
N	0.00000000	1.40494600	-0.40852700
O	0.00000000	-1.35323000	-0.42402300
Name of species: 3,7-di-H-PhozNH^{•+}			Y=H, radical cation
1 2			
C	-3.55574100	-0.74128400	-0.00021700
C	-2.35511000	-1.42014900	0.00000900
C	-1.17475100	-0.68869300	0.00008800
C	-1.19748500	0.71882000	0.00017400
C	-2.42679200	1.39436400	-0.00009400
C	-3.59063800	0.66533100	-0.00028400
C	1.19748500	0.71882000	0.00017400
C	1.17475100	-0.68869300	0.00008800
C	2.35511000	-1.42014900	0.00000900
H	2.30162300	-2.49904100	0.00006700
C	3.55574100	-0.74128400	-0.00021700
C	3.59063800	0.66533100	-0.00028400
C	2.42679200	1.39436400	-0.00009400
H	-4.48172100	-1.29746400	-0.00034200
H	-2.30162300	-2.49904100	0.00006700
H	-2.44301400	2.47595400	-0.00019300
H	-4.54185800	1.17671000	-0.00060600
H	0.00000000	2.39101700	0.00173600
H	4.48172100	-1.29746400	-0.00034200
H	4.54185800	1.17671000	-0.00060600
H	2.44301400	2.47595400	-0.00019300
N	0.00000000	1.37935500	0.00025100
O	0.00000000	-1.36243500	0.00031700
Name of species: 3,7-di-H-PhozN[•]			Y=H, radical
0 2			
C	-3.55700000	0.70439200	-0.00001400
C	-2.35291000	1.39025500	-0.00000700
C	-1.16749400	0.67325000	0.00001000
C	-1.14906100	-0.73789400	0.00001800
C	-2.39264500	-1.40295200	0.00001700
C	-3.57443200	-0.69603800	-0.00000100
C	1.14906100	-0.73789400	0.00000800
C	1.16749400	0.67325000	0.00000300
C	2.35291000	1.39025400	-0.00001800
H	2.30959800	2.46997400	-0.00002100
C	3.55700000	0.70439100	-0.00003500
C	3.57443200	-0.69603800	-0.00002800
C	2.39264500	-1.40295200	-0.00000600
H	-4.48542500	1.25722400	-0.00002900
H	-2.30959800	2.46997400	-0.00001600
H	-2.37195300	-2.48350500	0.00002600
H	-4.51822700	-1.22222100	-0.00000300
H	4.48542500	1.25722400	-0.00005300

H	4.51822700	-1.22222100	-0.00003900
H	2.37195300	-2.48350500	0.00000000
N	0.00000000	-1.46251000	0.00002800
O	0.00000000	1.37781000	0.00003200
Name of species: 3,7-di-H-PhozN⁻			Y=H, Anion
-1 1			
C	3.59382200	0.71719300	0.00001100
C	2.35584000	1.37591200	0.00000600
C	1.18177000	0.65958000	-0.00001000
C	1.14642000	-0.75927000	-0.00001800
C	2.40721400	-1.38814300	-0.00001300
C	3.59983800	-0.67105600	0.00000100
C	-1.14642000	-0.75927000	-0.00001100
C	-1.18177000	0.65958000	-0.00000200
C	-2.35584000	1.37591200	0.00002200
H	-2.29037500	2.45684900	0.00002700
C	-3.59382200	0.71719300	0.00003600
C	-3.59983800	-0.67105600	0.00002500
C	-2.40721400	-1.38814300	0.00000400
H	4.51506300	1.28323700	0.00002200
H	2.29037500	2.45684900	0.00001100
H	2.40591600	-2.47046100	-0.00002000
H	4.54092700	-1.20813500	0.00000400
H	-4.51506300	1.28323700	0.00005300
H	-4.54092700	-1.20813500	0.00003400
H	-2.40591600	-2.47046100	-0.00000300
N	0.00000000	-1.48720200	-0.00002900
O	0.00000000	1.38460600	-0.00002900
Name of species: 3,7-di-F-PhozNH			Y=F, neutral
Cartesian Coordinates			
0 1			
C	3.49589900	-0.53554400	0.17486700
C	2.31118000	-1.20027400	-0.08733000
C	1.16869300	-0.44572100	-0.26580100
C	1.19366600	0.94666800	-0.17144700
C	2.39904600	1.57488200	0.10814700
C	3.56651200	0.83640800	0.27745000
C	-1.19366500	0.94667000	-0.17145100
C	-1.16869800	-0.44572000	-0.26579900
C	-2.31117900	-1.20027600	-0.08732100
H	-2.27527900	-2.27674500	-0.16193600
C	-3.49590100	-0.53554400	0.17486900
C	-3.56651300	0.83640700	0.27744000
C	-2.39904700	1.57488300	0.10813500
H	2.27528600	-2.27674300	-0.16195200
H	2.42965600	2.65394200	0.18210000
H	4.51210200	1.31357100	0.48568500
H	-4.51210200	1.31357600	0.48566600
H	-2.42966500	2.65394300	0.18207700
N	0.00000200	1.64716400	-0.39765200
O	0.00000100	-1.10564200	-0.57884000
F	4.61828700	-1.26622700	0.33735800

F	-4.61828600	-1.26622800	0.33736600
H	0.00000000	2.60849800	-0.10043000
Name of species: 3,7-di-F-PhozNH^{•+}			Y=F, radical cation
Cartesian Coordinates			
1 2			
C	-3.53269700	0.52288100	-0.00002000
C	-2.34690000	1.22480000	0.00000100
C	-1.17465000	0.49001900	0.00002400
C	-1.19717800	-0.91823100	0.00002600
C	-2.42773700	-1.59377600	0.00000500
C	-3.59652900	-0.87582900	-0.00001700
C	1.19717800	-0.91823100	0.00002200
C	1.17465000	0.49001900	0.00002100
C	2.34690000	1.22480000	-0.00000200
H	2.32863100	2.30443800	0.00000000
C	3.53269700	0.52288100	-0.00002400
C	3.59652900	-0.87582900	-0.00002700
C	2.42773700	-1.59377600	-0.00000400
H	-2.32863100	2.30443800	0.00000100
H	-2.44603000	-2.67513900	0.00000000
H	-4.56229300	-1.35895700	-0.00003600
H	4.56229300	-1.35895700	-0.00005000
H	2.44603000	-2.67513900	-0.00001100
N	0.00000000	-1.57970800	0.00004400
O	0.00000000	1.16548600	0.00006000
F	-4.66985700	1.19924700	-0.00004200
F	4.66985700	1.19924700	-0.00005100
H	0.00000000	-2.59143300	0.00011300
Name of species: 3,7-di-F-PhozN[•]			Y=F, radical
Cartesian Coordinates			
0 2			
C	-3.52845900	0.48793900	-0.00002900
C	-2.34602300	1.19812500	-0.00003200
C	-1.16637700	0.47445700	0.00000700
C	-1.14907600	-0.93681300	0.00004700
C	-2.39245600	-1.60026500	0.00005600
C	-3.57972400	-0.90133200	0.00001800
C	1.14907600	-0.93681300	0.00003900
C	1.16637700	0.47445700	0.00000100
C	2.34602300	1.19812500	-0.00004000
H	2.33755000	2.27748000	-0.00006700
C	3.52845900	0.48793900	-0.00004000
C	3.57972400	-0.90133200	0.00000100
C	2.39245600	-1.60026500	0.00004100
H	-2.33755000	2.27748000	-0.00006200
H	-2.37474800	-2.68046000	0.00009200
H	-4.53827000	-1.39786200	0.00002600
H	4.53827000	-1.39786200	0.00000300
H	2.37474800	-2.68046000	0.00007400
N	0.00000000	-1.66249000	0.00007700
O	0.00000000	1.17960900	0.00001800
F	-4.68416800	1.17427300	-0.00005600

F	4.68416800	1.17427300	-0.00007300
Name of species: 3,7-di-F-PhozN⁻			Y=F, anion
Cartesian Coordinates			
-1 1			
C	-3.55784100	-0.49286700	0.00028700
C	-2.34858200	-1.17707600	0.00004300
C	-1.17915200	-0.44861400	-0.00027300
C	-1.14720200	0.97010000	-0.00025100
C	-2.40822400	1.59345500	0.00001100
C	-3.60818800	0.87927000	0.00025500
C	1.14720200	0.97010000	-0.00025700
C	1.17915200	-0.44861400	-0.00027700
C	2.34858200	-1.17707600	0.00003800
H	2.31593000	-2.25720400	-0.00000900
C	3.55784100	-0.49286700	0.00028600
C	3.60818800	0.87927000	0.00025700
C	2.40822400	1.59345500	0.00000900
H	-2.31592900	-2.25720400	-0.00000400
H	-2.41475600	2.67487200	-0.00001100
H	-4.56396200	1.38451700	0.00042300
H	4.56396200	1.38451700	0.00042900
H	2.41475600	2.67487200	-0.00001000
N	0.00000000	1.69918100	-0.00050200
O	0.00000000	-1.17348200	-0.00088400
F	-4.72029400	-1.22233300	0.00049800
F	4.72029400	-1.22233300	0.00050300
Name of species: 3,7-di-Cl-PhozNH			Y=Cl, neutral
Cartesian Coordinates			
0 1			
C	3.50946600	-0.33230700	0.10094000
C	2.31222700	-0.97143300	-0.19595600
C	1.16931700	-0.21091000	-0.33272500
C	1.19373800	1.17448900	-0.16343100
C	2.40014300	1.78718900	0.14529100
C	3.56546700	1.03912000	0.27273400
C	-1.19370400	1.17445700	-0.16343100
C	-1.16933000	-0.21092400	-0.33280300
C	-2.31227800	-0.97142500	-0.19607500
H	-2.26001400	-2.04157300	-0.33043300
C	-3.50947300	-0.33229400	0.10094300
C	-3.56541700	1.03912000	0.27288800
C	-2.40007500	1.78716800	0.14542800
H	2.25990300	-2.04158700	-0.33023600
H	2.43237200	2.86056600	0.27876100
H	4.50420700	1.51859200	0.50524100
H	-4.50413300	1.51857600	0.50551700
H	-2.43224200	2.86053000	0.27903400
N	0.00002800	1.88242400	-0.33810600
O	-0.00000600	-0.85251100	-0.68196700
H	-0.00005000	2.83486000	-0.01421400
Cl	4.95858900	-1.28532700	0.26490900
Cl	-4.95862900	-1.28528200	0.26485500

Name of species: 3,7-di-Cl-PhozNH^{•+}				Y=Cl, radical cation
Cartesian Coordinates				
1 2				
C	3.55023700	-0.32878000	-0.00000200	
C	2.34830800	-1.01419500	0.00006700	
C	1.17501000	-0.28078600	0.00007600	
C	1.19632700	1.12666400	0.00001800	
C	2.42741300	1.79912800	-0.00004700	
C	3.59389500	1.07784800	-0.00005700	
C	-1.19632700	1.12666400	0.00001200	
C	-1.17501000	-0.28078600	0.00007200	
C	-2.34830800	-1.01419500	0.00006100	
H	-2.30803600	-2.09344700	0.00011000	
C	-3.55023800	-0.32878000	-0.00001400	
C	-3.59389500	1.07784800	-0.00007200	
C	-2.42741200	1.79912800	-0.00005900	
H	2.30803500	-2.09344700	0.00011200	
H	2.44924600	2.88056200	-0.00009700	
H	4.55115500	1.57747600	-0.00011100	
H	-4.55115500	1.57747600	-0.00013100	
H	-2.44924600	2.88056200	-0.00011100	
N	0.00000000	1.78810500	0.00002000	
O	0.00000000	-0.95731100	0.00017100	
H	0.00000000	2.79975400	0.00004000	
Cl	5.02162100	-1.20428600	-0.00004300	
Cl	-5.02162100	-1.20428600	-0.00005400	
Name of species: 3,7-di-Cl-PhozN[•]				Y=Cl, radical
Cartesian Coordinates				
0 2				
C	3.54165400	-0.29342400	-0.00003200	
C	2.34628500	-0.99218200	0.00017200	
C	1.16616200	-0.26974400	0.00021300	
C	1.14783300	1.14173800	0.00005000	
C	2.39147900	1.80427000	-0.00013000	
C	3.57620500	1.10324700	-0.00017200	
C	-1.14783300	1.14173800	0.00005100	
C	-1.16616200	-0.26974400	0.00021500	
C	-2.34628500	-0.99218200	0.00017600	
H	-2.32022400	-2.07155100	0.00029700	
C	-3.54165400	-0.29342400	-0.00002600	
C	-3.57620500	1.10324700	-0.00016600	
C	-2.39147900	1.80427000	-0.00012600	
H	2.32022400	-2.07155100	0.00029400	
H	2.37694400	2.88465600	-0.00024400	
H	4.52697800	1.61457400	-0.00032400	
H	-4.52697800	1.61457400	-0.00031700	
H	-2.37694400	2.88465600	-0.00024100	
N	0.00000000	1.86542900	0.00004400	
O	0.00000000	-0.97399900	0.00048500	
Cl	-5.03483200	-1.17788900	-0.00014200	
Cl	5.03483200	-1.17788900	-0.00015200	
Name of species: 3,7-di-Cl-PhozN⁻				Y=Cl, anion

Cartesian Coordinates				
-1 1				
C	3.56821200	-0.28873800	-0.00023500	
C	2.34922600	-0.96876300	0.00021200	
C	1.17937200	-0.24471100	0.00057000	
C	1.14538000	1.17399400	0.00037900	
C	2.40490900	1.80179600	-0.00006700	
C	3.60188300	1.09092700	-0.00035100	
C	-1.14538000	1.17399300	0.00038800	
C	-1.17937200	-0.24471200	0.00057900	
C	-2.34922600	-0.96876300	0.00022200	
H	-2.30489600	-2.04854300	0.00039800	
C	-3.56821200	-0.28873800	-0.00022700	
C	-3.60188300	1.09092700	-0.00034600	
C	-2.40490900	1.80179600	-0.00006200	
H	2.30489600	-2.04854300	0.00038700	
H	2.40976200	2.88326900	-0.00017900	
H	4.55016100	1.61007100	-0.00068100	
H	-4.55016200	1.61007100	-0.00067800	
H	-2.40976200	2.88326900	-0.00017600	
N	0.00000000	1.90079800	0.00059900	
O	0.00000000	-0.96929200	0.00145700	
Cl	-5.06829900	-1.21220300	-0.00062500	
Cl	5.06829900	-1.21220300	-0.00062800	
Name of species: 3,7-di-CH₃-PhozNH			Y=CH ₃ , neutral	
Cartesian Coordinates				
0 1				
C	-3.53578200	-0.53380800	0.17097600	
C	-2.31562800	-1.15380500	-0.10909200	
C	-1.17078600	-0.40555400	-0.28241500	
C	-1.19341800	0.98594600	-0.16904000	
C	-2.39907900	1.60450400	0.12367000	
C	-3.55853300	0.85014600	0.28476500	
C	1.19341800	0.98594600	-0.16904000	
C	1.17078600	-0.40555400	-0.28241600	
C	2.31562800	-1.15380500	-0.10909300	
H	2.24303400	-2.22941700	-0.20517500	
C	3.53578200	-0.53380800	0.17097400	
C	3.55853300	0.85014600	0.28476400	
C	2.39907900	1.60450400	0.12366900	
H	-2.24303300	-2.22941700	-0.20517300	
H	-2.43294900	2.68280400	0.21547400	
H	-4.49041700	1.35359600	0.50477700	
H	0.00000000	2.64729700	-0.07712300	
H	4.49041700	1.35359600	0.50477500	
H	2.43294900	2.68280400	0.21547300	
N	0.00000000	1.68836100	-0.38176500	
O	0.00000000	-1.05974100	-0.61008900	
C	4.78341900	-1.36011000	0.33979900	
H	5.03114200	-1.88530400	-0.58352900	
H	5.63031600	-0.73135000	0.60904400	
H	4.65300400	-2.10819400	1.12255400	

C	-4.78341900	-1.36011000	0.33979800
H	-4.65299300	-2.10821900	1.12252600
H	-5.63030900	-0.73135400	0.60907800
H	-5.03116100	-1.88527400	-0.58354300
Name of species: 3,7-di-CH₃-PhozNH^{•+}			Y= CH ₃ , radical cation
Cartesian Coordinates			
1 2			
C	-3.57255900	0.52550700	0.00000200
C	-2.35417100	1.18361400	0.00000000
C	-1.17578800	0.45264200	-0.00000200
C	-1.19622500	-0.95285800	-0.00000200
C	-2.43023900	-1.62076200	0.00000000
C	-3.58916100	-0.88847700	0.00000200
C	1.19622500	-0.95285800	-0.00000100
C	1.17578800	0.45264200	-0.00000200
C	2.35417100	1.18361400	0.00000000
H	2.29315100	2.26279900	-0.00000100
C	3.57255900	0.52550700	0.00000200
C	3.58916100	-0.88847700	0.00000300
C	2.43023900	-1.62076200	0.00000100
H	-2.29315100	2.26279900	-0.00000100
H	-2.45363800	-2.70234100	0.00000100
H	-4.54154600	-1.40073700	0.00000300
H	0.00000000	-2.62673700	-0.00000800
H	4.54154600	-1.40073700	0.00000400
H	2.45363800	-2.70234100	0.00000200
N	0.00000000	-1.61559000	-0.00000300
O	0.00000000	1.12900400	-0.00000600
C	4.86569500	1.28241400	0.00000200
H	5.45527300	1.02179400	0.87983100
H	5.45526900	1.02180100	-0.87983200
H	4.69814700	2.35612000	0.00000700
C	-4.86569500	1.28241400	0.00000500
H	-5.45527700	1.02179000	-0.87982000
H	-5.45526500	1.02180400	0.87984200
H	-4.69814700	2.35612000	-0.00000500
Name of species: 3,7-di-CH₃-PhozN[•]			Y= CH ₃ , radical
Cartesian Coordinates			
0 2			
C	3.57010400	-0.49135800	0.00027200
C	2.35248700	-1.15748800	0.00002700
C	1.16742500	-0.43850800	0.00004600
C	1.14761200	0.97041200	0.00016300
C	2.39632000	1.62650900	0.00058300
C	3.57266300	0.91462700	0.00072200
C	-1.14761200	0.97041200	-0.00012100
C	-1.16742500	-0.43850800	-0.00003800
C	-2.35248700	-1.15748700	-0.00006800
H	-2.30252200	-2.23797200	0.00001800
C	-3.57010500	-0.49135600	-0.00033300
C	-3.57266300	0.91462800	-0.00077000
C	-2.39632000	1.62651000	-0.00057100

H	2.30252100	-2.23797300	-0.00009700
H	2.38445500	2.70734700	0.00088200
H	4.51898600	1.43983300	0.00111900
H	-4.51898600	1.43983400	-0.00120500
H	-2.38445500	2.70734700	-0.00086000
N	0.00000000	1.69765200	0.00003500
O	0.00000000	-1.14522700	0.00000500
C	-4.86846500	-1.24950400	0.00085900
H	-5.45642200	-1.00376800	0.88630900
H	-5.46607400	-0.99065700	-0.87425400
H	-4.69639700	-2.32381900	-0.00786600
C	4.86846600	-1.24950300	-0.00083300
H	5.45703100	-1.00286300	-0.88562200
H	5.46547300	-0.99154600	0.87495900
H	4.69639500	-2.32382600	0.00670500
Name of species: 3,7-di-CH₃-PhozN⁻			Y= CH ₃ , anion
Cartesian Coordinates			
-1 1			
C	3.60239000	-0.49218700	0.00031800
C	2.35326700	-1.13560900	-0.00012400
C	1.18156900	-0.41653000	-0.00047500
C	1.14670400	1.00325200	-0.00030000
C	2.40947400	1.62164000	0.00014000
C	3.59966800	0.89511100	0.00040600
C	-1.14670200	1.00325000	-0.00029300
C	-1.18156900	-0.41652800	-0.00046800
C	-2.35326700	-1.13561100	-0.00010600
H	-2.28405100	-2.21774300	-0.00027700
C	-3.60238800	-0.49219200	0.00034600
C	-3.59966600	0.89510900	0.00044200
C	-2.40947600	1.62163900	0.00016700
H	2.28406000	-2.21774100	-0.00029500
H	2.42037200	2.70382000	0.00024000
H	4.54431300	1.42863100	0.00071700
H	-4.54431300	1.42862500	0.00077000
H	-2.42037000	2.70381900	0.00028300
N	0.00000000	1.73113700	-0.00050000
O	0.00000100	-1.14002000	-0.00128900
C	-4.87808500	-1.29357900	0.00062500
H	-4.95082400	-1.93789400	0.88123200
H	-5.74432100	-0.63064200	0.00101500
H	-4.95139700	-1.93760000	-0.88015000
C	4.87808100	-1.29358300	0.00066000
H	4.95120900	-1.93794300	-0.87988100
H	5.74432400	-0.63065500	0.00062800
H	4.95099000	-1.93756100	0.88150100
Name of species: 3,7-di-OCH₃-PhozNH			Y= OCH ₃ , neutral
Cartesian Coordinates			
0 1			
C	-3.51645000	-0.46484100	0.07874600
C	-2.30481200	-1.08427900	-0.23337900
C	-1.16913400	-0.32322700	-0.38331800

C	-1.19256700	1.06515800	-0.21612600
C	-2.39663000	1.66323600	0.10639800
C	-3.56485600	0.91192500	0.25046800
C	1.19256700	1.06515800	-0.21612800
C	1.16913400	-0.32322700	-0.38331900
C	2.30481200	-1.08427900	-0.23338100
H	2.26079400	-2.15524800	-0.36510000
C	3.51645000	-0.46484100	0.07874100
C	3.56485700	0.91192500	0.25046300
C	2.39663100	1.66323600	0.10639400
H	-2.26079500	-2.15524800	-0.36509800
H	-2.43521100	2.73702500	0.23824100
H	-4.48585900	1.41727600	0.49374100
H	0.00000000	2.71772900	-0.05554500
H	4.48586100	1.41727700	0.49373500
H	2.43521200	2.73702500	0.23823700
N	0.00000000	1.77933100	-0.41895600
O	0.00000000	-0.96193700	-0.73848800
O	-4.58887800	-1.29695900	0.19548000
O	4.58887900	-1.29695900	0.19547400
C	-5.83449800	-0.70752600	0.51728900
H	-6.54760400	-1.52389800	0.56948300
H	-5.78818000	-0.20011000	1.48321500
H	-6.14372800	-0.00081600	-0.25577000
C	5.83449500	-0.70752700	0.51729800
H	6.54760100	-1.52390000	0.56950000
H	6.14373600	-0.00081700	-0.25575700
H	5.78816700	-0.20011100	1.48322400
Name of species: 3,7-di-OCH₃-PhozNH^{•+}			Y= OCH ₃ , radical cation
Cartesian Coordinates			
1 2			
C	3.56814400	-0.44975300	-0.00000200
C	2.34442100	-1.12580700	-0.00001400
C	1.17813700	-0.40300400	-0.00002000
C	1.19620300	1.00824600	-0.00001200
C	2.42740000	1.67389600	-0.00000100
C	3.60278400	0.96120500	0.00000200
C	-1.19620300	1.00824600	-0.00000800
C	-1.17813700	-0.40300300	-0.00001700
C	-2.34442100	-1.12580700	-0.00001100
H	-2.32186100	-2.20528900	-0.00001800
C	-3.56814400	-0.44975200	0.00000300
C	-3.60278400	0.96120600	0.00001000
C	-2.42739900	1.67389600	0.00000600
H	2.32186100	-2.20529000	-0.00002000
H	2.44784900	2.75564800	0.00000400
H	4.54229200	1.49009800	0.00000800
H	0.00000000	2.68166200	-0.00001800
H	-4.54229100	1.49009900	0.00001800
H	-2.44784900	2.75564900	0.00001300
N	0.00000100	1.67095400	-0.00001400
O	0.00000000	-1.08190400	-0.00004300

O	4.65088100	-1.21935000	0.00000100
O	-4.65088100	-1.21935000	0.00000300
C	5.94844900	-0.61269100	0.00002900
H	6.64972500	-1.43828500	0.00005100
H	6.08488700	-0.01074900	-0.89762500
H	6.08484400	-0.01073700	0.89768100
C	-5.94844900	-0.61269200	0.00005300
H	-6.64972500	-1.43828600	0.00008200
H	-6.08483100	-0.01074200	0.89771100
H	-6.08490200	-0.01074500	-0.89759500
Name of species: 3,7-di-OCH₃-PhozN[•]			Y= OCH ₃ , radical
Cartesian Coordinates			
0 2			
C	3.55940200	-0.42646100	0.00002200
C	2.34320000	-1.10841600	-0.00001400
C	1.16870300	-0.39067100	-0.00002500
C	1.14809300	1.02378500	0.00000300
C	2.39305500	1.67390600	0.00003900
C	3.58453000	0.97387500	0.00005100
C	-1.14809400	1.02378300	0.00000300
C	-1.16870200	-0.39067300	-0.00002200
C	-2.34319900	-1.10841800	-0.00000700
H	-2.32677400	-2.18811500	-0.00002700
C	-3.55940100	-0.42646400	0.00002900
C	-3.58453200	0.97387100	0.00005000
C	-2.39305700	1.67390300	0.00003600
H	2.32677600	-2.18811200	-0.00003900
H	2.38321300	2.75465800	0.00006500
H	4.51762500	1.51470900	0.00009000
H	-4.51762800	1.51470300	0.00008200
H	-2.38321700	2.75465500	0.00005600
N	-0.00000100	1.75069400	0.00000200
O	0.00000100	-1.09573900	-0.00007300
O	4.66662500	-1.20659200	0.00003700
O	-4.66662500	-1.20659400	0.00004900
C	5.93151300	-0.56447100	-0.00010100
H	6.66772100	-1.36135300	-0.00020100
H	6.05541600	0.04957600	-0.89370000
H	6.05563100	0.04954700	0.89348800
C	-5.93150900	-0.56446700	-0.00002800
H	-6.66772200	-1.36134500	-0.00008200
H	-6.05557700	0.04956000	0.89356100
H	-6.05545500	0.04957200	-0.89362600
Name of species: 3,7-di-OCH₃-PhozN⁻			Y= OCH ₃ , anion
Cartesian Coordinates			
-1 1			
C	3.56398700	-0.28916600	-0.34164000
C	2.34155600	-0.95700600	-0.22222700
C	1.17532700	-0.23407700	-0.11298600
C	1.14183300	1.18490000	-0.11192600
C	2.39697400	1.80912400	-0.24019400
C	3.58775900	1.09188200	-0.35056300

C	-1.14163100	1.18491700	0.10898100
C	-1.17541300	-0.23404500	0.10711900
C	-2.34137400	-0.95699100	0.21917900
H	-2.29906000	-2.03850400	0.22207400
C	-3.56330400	-0.28916000	0.34366100
C	-3.58682900	1.09186900	0.35499900
C	-2.39625400	1.80912000	0.24242200
H	2.29908400	-2.03850200	-0.22761700
H	2.40082300	2.89088600	-0.25259000
H	4.53646200	1.60353900	-0.45475000
H	-4.53514400	1.60345500	0.46296600
H	-2.39986800	2.89085700	0.25692600
N	0.00003300	1.91320700	-0.00222000
O	-0.00043700	-0.95930200	-0.00708100
O	4.74384200	-1.02442100	-0.45329100
O	-4.74297500	-1.02436600	0.45764700
C	5.26703300	-1.38518000	0.81200600
H	6.17637900	-1.95853300	0.63507300
H	5.50121900	-0.49330000	1.40001600
H	4.55070700	-1.99498300	1.36945300
C	-5.26919200	-1.38434500	-0.80661300
H	-6.17800400	-1.95797800	-0.62784600
H	-5.50496200	-0.49208900	-1.39342200
H	-4.55415500	-1.99363800	-1.36625300
Name of species: 3,7-di-NH₂-PhozNH			Y= NH ₂ , neutral
Cartesian Coordinates			
0 1			
C	3.53086200	-0.54948100	-0.17735100
C	2.30950900	-1.17175000	0.08974100
C	1.16960400	-0.41414900	0.26692200
C	1.19177700	0.97609600	0.17155000
C	2.40403100	1.58693600	-0.11165800
C	3.56367300	0.83935600	-0.28097100
C	-1.19177600	0.97609500	0.17155000
C	-1.16960400	-0.41414900	0.26692100
C	-2.30951000	-1.17175000	0.08974200
H	-2.22997000	-2.24807000	0.16242900
C	-3.53086100	-0.54948200	-0.17735100
C	-3.56367200	0.83935600	-0.28097300
C	-2.40403100	1.58693600	-0.11166000
H	2.22996900	-2.24807000	0.16242400
H	2.44610200	2.66613500	-0.18896100
H	4.49661900	1.34073400	-0.50095700
H	0.00000000	2.62838200	0.04654400
H	-4.49661800	1.34073200	-0.50096300
H	-2.44610000	2.66613500	-0.18896300
N	0.00000000	1.68776300	0.40517500
O	0.00000000	-1.07758100	0.57739500
N	4.68025100	-1.31777200	-0.39856000
H	5.54437900	-0.82949500	-0.23371700
H	4.67392500	-2.21798300	0.05077400
N	-4.68025400	-1.31777000	-0.39856100

H	-4.67391800	-2.21798900	0.05075700
H	-5.54437800	-0.82949700	-0.23368400
Name of species: 3,7-di-NH₂-PhozNH^{•+}			Y= NH ₂ , radical cation
Cartesian Coordinates			
1 2			
C	-3.57911800	-0.53093000	0.00002700
C	-2.34309900	-1.19667300	-0.00001900
C	-1.18013200	-0.46709600	-0.00004700
C	-1.19595100	0.94078800	-0.00002500
C	-2.43270400	1.60209300	0.00002100
C	-3.59950400	0.88677200	0.00004800
C	1.19595500	0.94078700	-0.00003300
C	1.18013900	-0.46708900	-0.00004300
C	2.34310200	-1.19666900	-0.00001000
H	2.28336300	-2.27554900	-0.00003800
C	3.57912200	-0.53092200	0.00003600
C	3.59950400	0.88677200	0.00003100
C	2.43269600	1.60209500	-0.00000100
H	-2.28335700	-2.27555300	-0.00003800
H	-2.45784300	2.68376100	0.00003400
H	-4.54851300	1.40386300	0.00008600
H	-0.00000200	2.61496400	-0.00002500
H	4.54850600	1.40387400	0.00005600
H	2.45784100	2.68376200	0.00000200
N	-0.00000800	1.60512200	-0.00004900
O	-0.00000200	-1.14925600	-0.00012600
N	-4.73760200	-1.22424600	0.00009700
H	-5.62326600	-0.75283900	-0.00004400
H	-4.74486600	-2.22767500	-0.00011200
N	4.73760500	-1.22424800	0.00006100
H	4.74485600	-2.22767700	0.00024000
H	5.62327200	-0.75284800	0.00017000
Name of species: 3,7-di-NH₂-PhozN[•]			Y= NH ₂ , radical
Cartesian Coordinates			
0 2			
C	3.56841800	-0.50066200	-0.00354600
C	2.34407800	-1.17101100	-0.01069400
C	1.16931000	-0.44655600	-0.00782700
C	1.14719600	0.96439200	0.00008300
C	2.39844000	1.61146300	0.00399400
C	3.57878900	0.90544100	0.00013600
C	-1.14719500	0.96439200	0.00008600
C	-1.16931000	-0.44655400	-0.00782500
C	-2.34407900	-1.17101000	-0.01070200
H	-2.29350600	-2.25132000	-0.02338100
C	-3.56841700	-0.50066300	-0.00355200
C	-3.57878600	0.90544100	0.00013500
C	-2.39844000	1.61146400	0.00399500
H	2.29350900	-2.25132000	-0.02334900
H	2.39232800	2.69238300	0.00909300
H	4.52571600	1.42892000	-0.00411500
H	-4.52571600	1.42891600	-0.00410900

H	-2.39232500	2.69238400	0.00909100
N	0.00000100	1.69191200	0.00504700
O	0.00000000	-1.15376200	-0.01217600
N	4.75873100	-1.20983200	-0.05255100
H	5.57631600	-0.72087500	0.26766400
H	4.72040700	-2.16534600	0.25676000
N	-4.75874000	-1.20983600	-0.05257000
H	-4.72040300	-2.16531500	0.25685800
H	-5.57628800	-0.72086700	0.26773800
Name of species: 3,7-di-NH₂-PhozN⁻			Y= NH ₂ , anion
Cartesian Coordinates			
-1 1			
C	3.59130700	-0.50657600	0.00168900
C	2.34839300	-1.15196900	-0.03879200
C	1.18058800	-0.42292900	-0.03290200
C	1.14712300	0.99554900	-0.01091700
C	2.41222500	1.60570100	0.01198300
C	3.60450700	0.87782300	0.02682200
C	-1.14716600	0.99555400	-0.01091300
C	-1.18057100	-0.42298000	-0.03292500
C	-2.34836500	-1.15198600	-0.03883300
H	-2.28460100	-2.23215500	-0.08937600
C	-3.59129400	-0.50655000	0.00169300
C	-3.60452800	0.87780900	0.02689100
C	-2.41222600	1.60571200	0.01208700
H	2.28455000	-2.23213400	-0.08934100
H	2.42980500	2.68762500	0.02831800
H	4.55193800	1.40592800	0.06039000
H	-4.55197000	1.40589500	0.06054000
H	-2.42978900	2.68763300	0.02851100
N	-0.00001100	1.72690600	-0.01058600
O	-0.00000100	-1.14623800	-0.07360800
N	4.79173800	-1.28730900	-0.03127600
H	5.59903800	-0.69940400	0.11428300
H	4.78492800	-1.99547300	0.68931400
N	-4.79170900	-1.28735200	-0.03136600
H	-4.78498800	-1.99530300	0.68944600
H	-5.59898800	-0.69937600	0.11408200
Name of species: 3,7-di-CF₃-PhozNH			Y= CF ₃ , neutral
Cartesian Coordinates			
0 1			
C	-3.52552100	-0.03448900	-0.00341900
C	-2.31741100	-0.66903700	-0.28223600
C	-1.16880500	0.08441900	-0.37064000
C	-1.19586100	1.46687300	-0.16610300
C	-2.40627800	2.08332500	0.12355700
C	-3.57364500	1.33542100	0.20057000
C	1.19523000	1.46932200	-0.14392600
C	1.17369700	0.08593900	-0.35028000
C	2.32000000	-0.66535600	-0.23404500
H	2.26848200	-1.73330300	-0.39232200
C	3.52135000	-0.02981400	0.07584400

C	3.56498400	1.33937600	0.27687600
C	2.39712200	2.08591400	0.17548900
H	-2.26168500	-1.73482900	-0.45042400
H	-2.43379000	3.15370200	0.27834200
H	-4.51474100	1.81993600	0.41371100
H	-0.00362700	3.12974700	0.02179100
H	4.49844900	1.82375800	0.51987600
H	2.41891700	3.15515300	0.33872600
N	0.00016400	2.17140800	-0.28361400
O	0.00607800	-0.54878200	-0.71387900
C	4.76535300	-0.85488100	0.13747300
C	-4.76366800	-0.85831800	0.14273900
F	5.77949400	-0.20354700	0.72864900
F	4.57028600	-1.99967300	0.81809800
F	5.19192700	-1.21238100	-1.09083600
F	-4.75482100	-1.92820400	-0.67095300
F	-5.87450400	-0.15285300	-0.13007200
F	-4.90583400	-1.33177700	1.39791600
Name of species: 3,7-di-CF₃-PhozNH⁺			Y= CF ₃ , radical cation
Cartesian Coordinates			
1 2			
C	-3.54329700	-0.06932100	-0.00791500
C	-2.35139900	-0.75496000	-0.00488200
C	-1.17262800	-0.01715100	-0.00227200
C	-1.19674500	1.38932000	-0.00208700
C	-2.42702600	2.06572600	-0.00491500
C	-3.58844800	1.33816800	-0.00764800
C	1.19674400	1.38932500	0.00209300
C	1.17263500	-0.01714700	0.00231200
C	2.35140800	-0.75494700	0.00494500
H	2.30711600	-1.83445000	0.00557900
C	3.54330600	-0.06930000	0.00797000
C	3.58844800	1.33818500	0.00766900
C	2.42701800	2.06573700	0.00491600
H	-2.30709900	-1.83446300	-0.00549200
H	-2.44641200	3.14707300	-0.00533900
H	-4.54603200	1.83998900	-0.01088000
H	-0.00000600	3.06243700	-0.00005800
H	4.54602600	1.84001500	0.01089700
H	2.44640200	3.14708400	0.00531800
N	-0.00000300	2.05014300	-0.00001200
O	0.00000300	-0.69044200	0.00000400
C	4.85540800	-0.81317400	-0.00059400
C	-4.85540600	-0.81318000	0.00058100
F	5.60709900	-0.43795400	1.03947900
F	4.67373000	-2.13205000	0.06309900
F	5.53585600	-0.53328100	-1.11749300
F	-4.67373100	-2.13207800	-0.06249300
F	-5.60678700	-0.43839100	-1.03987100
F	-5.53617800	-0.53278300	1.11716700
Name of species: 3,7-di-CF₃-PhozN[•]			Y= CF ₃ , radical
Cartesian Coordinates			

0 2			
C	-3.54245800	-0.04314800	-0.01043500
C	-2.34868500	-0.73968100	-0.00565300
C	-1.16507500	-0.01847400	-0.00278000
C	-1.14754900	1.39201500	-0.00292400
C	-2.39055900	2.06191600	-0.00725100
C	-3.56969800	1.35905700	-0.01086900
C	1.14755200	1.39202600	0.00279100
C	1.16509200	-0.01846400	0.00264200
C	2.34870700	-0.73965600	0.00566800
H	2.31641200	-1.81892600	0.00570800
C	3.54247800	-0.04311000	0.01068300
C	3.56970400	1.35909200	0.01110000
C	2.39055300	2.06193700	0.00727400
H	-2.31637500	-1.81895100	-0.00565300
H	-2.37004000	3.14202900	-0.00821700
H	-4.51907900	1.87562100	-0.01547000
H	4.51907200	1.87567300	0.01590800
H	2.37002400	3.14205000	0.00825100
N	-0.00000200	2.11438200	-0.00010000
O	0.00001200	-0.72196300	-0.00013700
C	4.84928000	-0.77346700	-0.00081300
C	-4.84928200	-0.77346800	0.00089100
F	5.63034600	-0.39844500	1.02841900
F	4.69395000	-2.10245800	0.07593400
F	5.54500000	-0.51479200	-1.12378900
F	-4.69390000	-2.10259100	-0.07343800
F	-5.62922600	-0.40020000	-1.02984400
F	-5.54622200	-0.51283800	1.12264300
Name of species: 3,7-di-CF₃-PhozN⁻		Y= CF ₃ , anion	
Cartesian Coordinates			
-1 1			
C	-3.58215000	0.00336600	0.00285500
C	-2.35226700	-0.67704200	-0.00055600
C	-1.18148300	0.03255400	0.00459400
C	-1.14482100	1.45471000	0.01128600
C	-2.39890500	2.09605000	0.01454800
C	-3.59306900	1.39097700	0.01065400
C	1.14392600	1.45139500	0.00033200
C	1.17743400	0.02999500	-0.00557000
C	2.34636600	-0.68341900	-0.02797200
H	2.29928100	-1.76397800	-0.03829500
C	3.57727000	-0.00665900	-0.04643600
C	3.59135100	1.38187400	-0.03250200
C	2.40012100	2.08997600	-0.01382300
H	-2.30815400	-1.75823800	-0.00558700
H	-2.39200500	3.17713500	0.02006200
H	-4.53433400	1.92186000	0.01349200
H	4.53433400	1.91010300	-0.04481800
H	2.39572000	3.17110200	-0.01271400
N	0.00073200	2.17362000	0.01327300
O	-0.00301100	-0.68880400	0.00832400

C	4.82818200	-0.78794800	-0.00105000
C	-4.82834800	-0.78665500	-0.00299000
F	5.11718700	-1.28609100	1.23502800
F	4.80168400	-1.87584200	-0.81170800
F	5.91514200	-0.06774600	-0.36016600
F	-4.93673000	-1.60861700	-1.08215500
F	-5.94178000	-0.02185200	-0.00243000
F	-4.94189300	-1.61740100	1.06900100
Name of species: 3,7-di-CN-PhozNH			Y= CN, neutral
Cartesian Coordinates			
0 1			
C	-3.58020900	-0.36338700	0.00028100
C	-2.35299600	-1.03516900	-0.00031900
C	-1.18333900	-0.31195300	-0.00066800
C	-1.20424700	1.08783200	-0.00034100
C	-2.42950900	1.74503300	0.00031100
C	-3.61576900	1.02731700	0.00058700
C	1.20424700	1.08783200	-0.00034200
C	1.18333900	-0.31195300	-0.00066800
C	2.35299600	-1.03516900	-0.00031900
H	2.30449700	-2.11415300	-0.00059000
C	3.58020900	-0.36338700	0.00028000
C	3.61576900	1.02731800	0.00058600
C	2.42950900	1.74503300	0.00031000
H	-2.30449700	-2.11415300	-0.00059000
H	-2.44923900	2.82658100	0.00057400
H	-4.56463100	1.54225800	0.00105800
H	4.56463100	1.54225900	0.00105600
H	2.44923800	2.82658100	0.00057300
N	0.00000000	1.76964100	-0.00071700
O	0.00000000	-1.01550300	-0.00155000
H	0.00000000	2.77365200	-0.00054000
C	-4.79925800	-1.11381200	0.00056200
N	-5.77916900	-1.71263000	0.00078200
C	4.79925800	-1.11381100	0.00056200
N	5.77916900	-1.71263100	0.00078200
Name of species: 3,7-di-CN-PhozNH^{•+}			Y= CN, radical cation
Cartesian Coordinates			
1 2			
C	-3.55253800	-0.37395700	0.00000100
C	-2.34878600	-1.05976100	-0.00002600
C	-1.17362300	-0.32573500	-0.00003400
C	-1.19662700	1.08271700	-0.00001400
C	-2.42558500	1.76019500	0.00001400
C	-3.59079300	1.03813300	0.00001900
C	1.19662700	1.08271700	-0.00000500
C	1.17362300	-0.32573500	-0.00002800
C	2.34878700	-1.05976100	-0.00001800
H	2.30695800	-2.13923400	-0.00003900
C	3.55253800	-0.37395700	0.00001900
C	3.59079300	1.03813300	0.00004500
C	2.42558400	1.76019500	0.00003400

H	-2.30695800	-2.13923400	-0.00004100
H	-2.44423500	2.84159200	0.00003400
H	-4.54683800	1.54047300	0.00004000
H	4.54683800	1.54047300	0.00007600
H	2.44423500	2.84159200	0.00005900
N	0.00000000	1.74196000	-0.00002000
O	0.00000000	-0.99950000	-0.00008000
H	0.00000000	2.75453900	-0.00006400
C	-4.78134500	-1.10625000	0.00001200
N	-5.77020500	-1.68728800	0.00002000
C	4.78134500	-1.10625000	0.00003100
N	5.77020500	-1.68728800	0.00004000
Name of species: 3,7-di-CN-PhozN[•]			Y= CN, radical
Cartesian Coordinates			
0 2			
C	-3.55012100	-0.34033100	-0.00000100
C	-2.34632000	-1.03816100	-0.00000400
C	-1.16577000	-0.32056200	-0.00000400
C	-1.14728700	1.09274800	0.00000000
C	-2.38881800	1.76434600	0.00000300
C	-3.57092700	1.06616000	0.00000300
C	1.14728700	1.09274800	0.00000100
C	1.16577000	-0.32056200	-0.00000300
C	2.34632000	-1.03816100	-0.00000300
H	2.31898900	-2.11774200	-0.00000600
C	3.55012100	-0.34033100	0.00000100
C	3.57092700	1.06616000	0.00000600
C	2.38881800	1.76434600	0.00000600
H	-2.31898900	-2.11774200	-0.00000700
H	-2.36690600	2.84440400	0.00000700
H	-4.51930800	1.58223700	0.00000500
H	4.51930800	1.58223700	0.00000900
H	2.36690600	2.84440400	0.00000900
N	0.00000000	1.81183600	0.00000200
O	0.00000000	-1.02262600	-0.00000900
C	-4.78356600	-1.06629100	-0.00000100
N	-5.77596400	-1.64389600	-0.00000100
C	4.78356600	-1.06629100	0.00000100
N	5.77596400	-1.64389600	0.00000100
Name of species: 3,7-di-CN-PhozN⁻			Y= CN, anion
Cartesian Coordinates			
-1 1			
C	-3.58474900	-0.34296700	0.00020900
C	-2.34924100	-1.02246700	-0.00023100
C	-1.17946000	-0.31204500	-0.00049800
C	-1.14337300	1.10907000	-0.00023900
C	-2.39791300	1.75505600	0.00019000
C	-3.58841300	1.05391200	0.00039000
C	1.14337300	1.10907000	-0.00023600
C	1.17946000	-0.31204500	-0.00049600
C	2.34924100	-1.02246700	-0.00023000
H	2.30866400	-2.10261500	-0.00044800

C	3.58474900	-0.34296700	0.00021400
C	3.58841300	1.05391300	0.00039800
C	2.39791300	1.75505600	0.00019800
H	-2.30866400	-2.10261600	-0.00044600
H	-2.38789100	2.83603900	0.00035500
H	-4.53182000	1.58233800	0.00070900
H	4.53182000	1.58233800	0.00072000
H	2.38789100	2.83603900	0.00036500
N	0.00000000	1.82852000	-0.00033200
O	0.00000000	-1.03201600	-0.00128700
C	-4.80687000	-1.07109800	0.00041800
N	-5.79973300	-1.65775600	0.00059000
C	4.80687000	-1.07109700	0.00042300
N	5.79973200	-1.65775700	0.00059400
Name of species: 3,7-di-NO₂-PhozNH			Y= NO ₂ , neutral
Cartesian Coordinates			
0 1			
C	3.51931100	-0.18991700	-0.06193000
C	2.32538200	-0.86460900	0.16461800
C	1.17372600	-0.12269000	0.28276500
C	1.19729800	1.27150600	0.15709800
C	2.40707100	1.91520200	-0.07995200
C	3.58130500	1.18562300	-0.18532300
C	-1.19729700	1.27150600	0.15709600
C	-1.17372600	-0.12268900	0.28276300
C	-2.32538200	-0.86460800	0.16461400
H	-2.29903100	-1.93909600	0.26100400
C	-3.51931100	-0.18991700	-0.06193700
C	-3.58130300	1.18562400	-0.18533000
C	-2.40707000	1.91520300	-0.07995600
H	2.29903000	-1.93909600	0.26100700
H	2.42659100	2.99235700	-0.17578600
H	4.53046400	1.66622000	-0.36259300
H	-4.53046100	1.66622100	-0.36260200
H	-2.42658900	2.99235800	-0.17579000
N	0.00000100	1.96136400	0.29054800
O	0.00000000	-0.78195300	0.57108600
N	4.75422100	-0.97115700	-0.17526500
N	-4.75422100	-0.97115700	-0.17527400
O	5.78283000	-0.36468200	-0.37610700
O	4.66785300	-2.17291400	-0.06106500
O	-5.78283200	-0.36468300	-0.37610900
O	-4.66785700	-2.17291100	-0.06104300
H	0.00000100	2.94341800	0.07345400
Name of species: 3,7-di-NO₂-PhozNH⁺			Y= NO ₂ , radical cation
Cartesian Coordinates			
1 2			
C	3.52640800	-0.19029200	-0.00002700
C	2.34860800	-0.89528100	0.00007900
C	1.17199200	-0.15766000	0.00010400
C	1.19700800	1.25175500	0.00001000
C	2.42524400	1.93067000	-0.00008900

C	3.59248300	1.20892800	-0.00010200
C	-1.19700700	1.25175500	0.00001600
C	-1.17199100	-0.15766000	0.00011000
C	-2.34860800	-0.89528100	0.00009200
H	-2.33346200	-1.97578900	0.00014600
C	-3.52640700	-0.19029100	-0.00001000
C	-3.59248300	1.20892900	-0.00008500
C	-2.42524300	1.93067100	-0.00007600
H	2.33346200	-1.97578900	0.00012600
H	2.44311900	3.01200000	-0.00015900
H	4.55866600	1.69110800	-0.00016600
H	-4.55866500	1.69110900	-0.00014900
H	-2.44311800	3.01200000	-0.00014400
N	0.00000000	1.91094300	0.00003800
O	0.00000000	-0.82972800	0.00025700
N	4.79708400	-0.95736600	-0.00005500
N	-4.79708300	-0.95736500	-0.00002900
O	5.81255800	-0.31094300	0.00017900
O	4.70197400	-2.15727600	-0.00025400
O	-5.81256000	-0.31094400	0.00007400
O	-4.70197700	-2.15727600	-0.00018300
H	0.00000100	2.92375100	-0.00005000
Name of species: 3,7-di-NO₂-PhozN[•]			Y= NO ₂ , radical
Cartesian Coordinates			
0 2			
C	3.52609600	-0.16296700	-0.00008500
C	2.34544800	-0.88033100	-0.00009000
C	1.16472100	-0.16146100	-0.00004700
C	1.14713100	1.25302700	0.00000500
C	2.38738500	1.92815700	0.00001400
C	3.57191200	1.23305600	-0.00003000
C	-1.14713600	1.25302200	0.00003000
C	-1.16472000	-0.16146600	-0.00002100
C	-2.34544400	-0.88034200	-0.00003800
H	-2.34172600	-1.95946400	-0.00008000
C	-3.52609500	-0.16297900	-0.00000500
C	-3.57191600	1.23304200	0.00004700
C	-2.38739100	1.92814800	0.00006600
H	2.34173300	-1.95945500	-0.00013100
H	2.36327600	3.00799400	0.00005400
H	4.52777700	1.73251700	-0.00002500
H	-4.52778400	1.73249900	0.00007400
H	-2.36328700	3.00798600	0.00010500
N	-0.00000300	1.97080900	0.00004400
O	0.00000200	-0.86213300	-0.00006200
N	4.79170700	-0.91170000	-0.00013300
N	-4.79170600	-0.91170300	-0.00002200
O	5.81606400	-0.26864100	0.00021700
O	4.72499800	-2.11951300	0.00017000
O	-5.81604400	-0.26861800	-0.00001800
O	-4.72501200	-2.11951500	-0.00009300
Name of species: 3,7-di-NO₂-PhozN⁻			Y= NO ₂ , anion

Cartesian Coordinates			
-1 1			
C	-3.56470200	-0.16791100	0.00034000
C	-2.34839200	-0.87021100	-0.00006900
C	-1.17869200	-0.16371200	-0.00039400
C	-1.14236400	1.25964300	-0.00021400
C	-2.39310800	1.91697200	0.00017300
C	-3.58440900	1.22444600	0.00042000
C	1.14236200	1.25964200	-0.00018300
C	1.17869000	-0.16371200	-0.00036400
C	2.34839000	-0.87021200	-0.00000900
H	2.33410700	-1.94905300	-0.00015800
C	3.56470100	-0.16791200	0.00044700
C	3.58440800	1.22444500	0.00052100
C	2.39310700	1.91697200	0.00024200
H	-2.33410900	-1.94905300	-0.00021500
H	-2.37471900	2.99747900	0.00027600
H	-4.53351100	1.73770800	0.00071000
H	4.53351000	1.73770700	0.00084100
H	2.37471800	2.99747900	0.00034700
N	-0.00000100	1.97497700	-0.00033700
O	-0.00000100	-0.87948900	-0.00119900
N	-4.79648800	-0.89607400	0.00060300
N	4.79648900	-0.89607300	0.00074200
O	-5.84843900	-0.26955200	0.00017000
O	-4.75150500	-2.11838000	-0.00015200
O	5.84843800	-0.26954900	-0.00012600
O	4.75151300	-2.11837900	-0.00048500

Table S10. Optimized Cartesian Coordinates of all PhtzNHs compounds

3,7-di-Y-PhtzNH compounds			
Name of species: 3,7-di-H-PhtzNH			Y=H, neutral
Cartesian Coordinates			
0 1			
C	3.63513500	-0.35780900	-0.58706000
C	2.54082800	-1.18075300	-0.34993400
C	1.34382800	-0.64261300	0.10322000
C	1.21553200	0.73673200	0.27900000
C	2.30768200	1.55979500	0.01550300
C	3.51506100	1.01281400	-0.39683000
C	-1.21553200	0.73673200	0.27900000
C	-1.34382800	-0.64261300	0.10322000
C	-2.54082800	-1.18075300	-0.34993500
H	-2.61279400	-2.24934200	-0.50090300
C	-3.63513500	-0.35780900	-0.58706000
C	-3.51506100	1.01281400	-0.39683000
C	-2.30768200	1.55979500	0.01550300
H	2.61279400	-2.24934200	-0.50090300

H	2.20868400	2.63053600	0.14358900
H	4.35762800	1.66382800	-0.58339400
H	-4.35762800	1.66382800	-0.58339400
H	-2.20868400	2.63053600	0.14358900
N	0.00000000	1.27180600	0.72767100
S	0.00000000	-1.70227100	0.56647700
H	0.00000000	2.27602100	0.79958200
H	-4.56953300	-0.78516900	-0.92113200
H	4.56953300	-0.78516900	-0.92113300
Name of species: 3,7-di-H-PhtzNH^{•+}			Y=H, radical cation
Cartesian Coordinates			
1 2			
C	3.75360800	0.41296800	0.00002300
C	2.63410800	1.21029600	0.00000700
C	1.35812600	0.62874300	-0.00000700
C	1.22858600	-0.77329100	-0.00000300
C	2.38448300	-1.57342700	0.00001300
C	3.62504700	-0.98662200	0.00002500
C	-1.22858600	-0.77329100	-0.00000400
C	-1.35812600	0.62874300	-0.00000900
C	-2.63410800	1.21029600	0.00000300
H	-2.72619300	2.28814900	0.00000000
C	-3.75360800	0.41296800	0.00002000
C	-3.62504700	-0.98662200	0.00002400
C	-2.38448300	-1.57342700	0.00001300
H	4.73461000	0.86447400	0.00003500
H	2.72619300	2.28814900	0.00000500
H	2.28247100	-2.65082100	0.00001700
H	4.50949900	-1.60727700	0.00003800
H	0.00000000	-2.38895700	-0.00002000
H	-4.73461000	0.86447400	0.00003000
H	-4.50949900	-1.60727700	0.00003700
H	-2.28247100	-2.65082100	0.00001800
N	0.00000000	-1.37833400	-0.00001400
S	0.00000000	1.70151500	-0.00004300
Name of species: 3,7-di-H-PhtzN[•]			Y=H, radical
Cartesian Coordinates			
0 2			
C	-3.75136000	-0.36873100	0.00042600
C	-2.63248600	-1.17897100	0.00017700
C	-1.35455500	-0.61764100	-0.00010800
C	-1.17941900	0.78827000	-0.00010900
C	-2.35174900	1.58530700	0.00011900
C	-3.60575500	1.02543500	0.00037600
C	1.17941900	0.78827000	-0.00010500
C	1.35455500	-0.61764100	-0.00010300
C	2.63248600	-1.17897100	0.00018600
H	2.73914400	-2.25605500	0.00021600
C	3.75136000	-0.36873100	0.00044000
C	3.60575500	1.02543500	0.00039500
C	2.35174900	1.58530700	0.00013300
H	-4.73584700	-0.81391500	0.00065800

H	-2.73914400	-2.25605500	0.00020800
H	-2.20403100	2.65587000	0.00010500
H	-4.48128200	1.65956400	0.00055700
H	4.73584700	-0.81391500	0.00067500
H	4.48128200	1.65956500	0.00058100
H	2.20403100	2.65587000	0.00012100
N	0.00000000	1.45153600	-0.00026200
S	0.00000000	-1.71598100	-0.00076500
Name of species: 3,7-di-H-PhtzN⁻			Y=H, anion
Cartesian Coordinates			
-1 1			
C	0.37318400	0.44819700	3.70492400
C	1.16750100	0.30030800	2.56848300
C	0.61155500	-0.04890500	1.34854600
C	-0.79108800	-0.20074800	1.17035600
C	-1.56344800	-0.05687300	2.34920400
C	-1.00079400	0.24720700	3.57674500
C	-0.79108800	-0.20074800	-1.17035600
C	0.61155500	-0.04890500	-1.34854600
C	1.16750100	0.30030800	-2.56848300
H	2.24190900	0.42967700	-2.63137600
C	0.37318400	0.44819700	-3.70492400
C	-1.00079400	0.24720700	-3.57674500
C	-1.56344800	-0.05687300	-2.34920400
H	2.24190900	0.42967700	2.63137600
H	-2.63221300	-0.18890400	2.24126600
H	-1.64341000	0.34232600	4.44425500
H	-1.64341000	0.34232600	-4.44425500
H	-2.63221300	-0.18890400	-2.24126600
N	-1.43471700	-0.43211300	0.00000000
S	1.68202000	-0.48825400	0.00000000
H	0.81759900	0.70021600	-4.65787900
H	0.81759900	0.70021600	4.65787900
Name of species: 3,7-di-F-PhtzNH			Y=F, neutral
Cartesian Coordinates			
0 1			
C	3.59961400	-0.26441900	-0.42914900
C	2.53249900	-1.08517800	-0.12128200
C	1.34152400	-0.50096000	0.28920100
C	1.21372700	0.88871300	0.34468300
C	2.30225200	1.68390600	-0.00117700
C	3.51155900	1.11117100	-0.37337300
C	-1.21372700	0.88871200	0.34468400
C	-1.34152400	-0.50096000	0.28920100
C	-2.53249900	-1.08517800	-0.12128200
H	-2.63777400	-2.15858900	-0.18720500
C	-3.59961400	-0.26442000	-0.42914900
C	-3.51155800	1.11117100	-0.37337300
C	-2.30225200	1.68390600	-0.00117600
H	2.63777500	-2.15858900	-0.18720600
H	2.20679600	2.76158700	0.03072100
H	4.36905400	1.71534400	-0.63024800

H	-4.36905400	1.71534300	-0.63024900
H	-2.20679600	2.76158700	0.03072200
N	0.00000000	1.45659000	0.76485800
S	0.00000000	-1.51940900	0.83901100
H	0.00000000	2.46323800	0.75617800
F	-4.76490600	-0.83246000	-0.80376300
F	4.76490600	-0.83246100	-0.80376300
Name of species: 3,7-di-F-PhtzNH^{•+}			Y=F, radical cation
Cartesian Coordinates			
1 2			
C	3.72801400	0.26854700	0.00003200
C	2.62839000	1.08967600	0.00000800
C	1.35860700	0.50665900	-0.00001900
C	1.22830500	-0.89580800	-0.00002000
C	2.38385400	-1.70032200	0.00000500
C	3.62823400	-1.12703100	0.00002900
C	-1.22830500	-0.89580800	-0.00001900
C	-1.35860700	0.50665900	-0.00002000
C	-2.62839000	1.08967600	0.00000800
H	-2.75939900	2.16304000	0.00001000
C	-3.72801400	0.26854700	0.00003200
C	-3.62823400	-1.12703100	0.00003300
C	-2.38385400	-1.70032200	0.00000900
H	2.75939900	2.16304000	0.00001100
H	2.28086500	-2.77749500	0.00000700
H	4.52975200	-1.72242300	0.00005000
H	-4.52975200	-1.72242300	0.00005600
H	-2.28086500	-2.77749500	0.00001300
N	0.00000000	-1.50092900	-0.00004200
S	0.00000000	1.58505000	-0.00008200
F	4.93632300	0.81281300	0.00005700
F	-4.93632300	0.81281300	0.00006000
H	0.00000000	-2.51181200	-0.00006500
Name of species: 3,7-di-Cl-PhtzN[•]			Y=F, radical
Cartesian Coordinates			
0 2			
C	-3.72091400	0.23013900	-0.00004900
C	-2.62722200	1.06380100	-0.00006000
C	-1.35375600	0.49713800	0.00000000
C	-1.17959800	-0.90885000	0.00006300
C	-2.35062700	-1.70671300	0.00007400
C	-3.60964100	-1.15670300	0.00002000
C	1.17959800	-0.90885000	0.00006100
C	1.35375600	0.49713800	0.00000100
C	2.62722200	1.06380100	-0.00005600
H	2.77128100	2.13537100	-0.00010500
C	3.72091400	0.23013900	-0.00004700
C	3.60964100	-1.15670300	0.00001500
C	2.35062700	-1.70671300	0.00006800
H	-2.77128100	2.13537100	-0.00011200
H	-2.20420200	-2.77710800	0.00012400
H	-4.50269600	-1.76417700	0.00002700

H	4.50269600	-1.76417700	0.00002000
H	2.20420200	-2.77710800	0.00011500
N	0.00000000	-1.57275700	0.00010900
S	0.00000000	1.59892300	0.00003000
F	-4.94837000	0.77847800	-0.00010400
F	4.94837000	0.77847800	-0.00010100
Name of species: 3,7-di-F-PhtzN⁻			Y=F, anion
Cartesian Coordinates			
-1 1			
C	3.66496100	-0.25538500	-0.32661900
C	2.56113800	-1.06233700	-0.13306800
C	1.34462300	-0.47416500	0.18607900
C	1.16980700	0.93462700	0.24919900
C	2.34736800	1.69428300	0.05001500
C	3.57920300	1.11874300	-0.22403000
C	-1.16980700	0.93462700	0.24919900
C	-1.34462300	-0.47416500	0.18607900
C	-2.56113800	-1.06233700	-0.13306800
H	-2.65748900	-2.13818100	-0.19665000
C	-3.66496100	-0.25538500	-0.32661900
C	-3.57920300	1.11874300	-0.22403000
C	-2.34736800	1.69428300	0.05001500
H	2.65748800	-2.13818100	-0.19665000
H	2.24386800	2.76911000	0.11306100
H	4.46397600	1.72324500	-0.37082100
H	-4.46397600	1.72324500	-0.37082100
H	-2.24386800	2.76911000	0.11306100
N	0.00000000	1.59176000	0.45089300
S	0.00000000	-1.51434100	0.69747400
F	-4.87330600	-0.83835600	-0.61255100
F	4.87330600	-0.83835600	-0.61255100
Name of species: 3,7-di-Cl-PhtzNH			Y=Cl, neutral
Cartesian Coordinates			
0 1			
C	3.60975500	-0.16725000	-0.29533900
C	2.52948900	-0.93590500	0.11049500
C	1.34015500	-0.30834200	0.45461700
C	1.21338700	1.07819500	0.34898700
C	2.30366000	1.82655100	-0.08482200
C	3.50907900	1.21124400	-0.39040400
C	-1.21338700	1.07819600	0.34898700
C	-1.34015500	-0.30834200	0.45461700
C	-2.52948900	-0.93590500	0.11049400
H	-2.61625700	-2.01134300	0.17228300
C	-3.60975500	-0.16725000	-0.29533900
C	-3.50907900	1.21124400	-0.39040200
C	-2.30366100	1.82655100	-0.08482100
H	2.61625800	-2.01134300	0.17228400
H	2.21150700	2.90117500	-0.17735900
H	4.35891000	1.79422400	-0.71326400
H	-4.35891100	1.79422400	-0.71326100
H	-2.21150900	2.90117600	-0.17735600

N	0.00000000	1.69263300	0.68821100
S	0.00000000	-1.25194800	1.12923900
H	0.00000000	2.69193500	0.56612100
Cl	5.11312900	-0.95091900	-0.69815200
Cl	-5.11312800	-0.95091900	-0.69815200
Name of species: 3,7-di-Cl-PhtzNH^{•+}			Y=Cl, radical cation
Cartesian Coordinates			
1 2			
C	-3.74613300	-0.14045700	0.00002600
C	-2.62905700	-0.94682200	-0.00005400
C	-1.35876800	-0.36427700	-0.00006600
C	-1.22746200	1.03736900	0.00000700
C	-2.38422600	1.83797000	0.00008800
C	-3.62652000	1.26048800	0.00009600
C	1.22746200	1.03736900	0.00001000
C	1.35876900	-0.36427600	-0.00006400
C	2.62905700	-0.94682200	-0.00005100
H	2.73745900	-2.02278200	-0.00010300
C	3.74613300	-0.14045700	0.00003200
C	3.62652000	1.26048800	0.00010400
C	2.38422600	1.83797000	0.00009500
H	-2.73745900	-2.02278200	-0.00010500
H	-2.28530900	2.91563900	0.00014700
H	-4.51850100	1.86992000	0.00016000
H	4.51850100	1.86992000	0.00017100
H	2.28530900	2.91563900	0.00015600
N	0.00000000	1.64258400	0.00000500
S	0.00000000	-1.44272800	-0.00021900
H	0.00000000	2.65342800	0.00003800
Cl	-5.30969200	-0.84719600	0.00004500
Cl	5.30969200	-0.84719600	0.00005300
Name of species: 3,7-di-Cl-PhtzN[•]			Y=Cl, radical
Cartesian Coordinates			
0 2			
C	-3.73450900	-0.10362500	0.00002700
C	-2.62654000	-0.92634300	-0.00001100
C	-1.35308500	-0.35989700	-0.00004800
C	-1.17819300	1.04600800	-0.00004000
C	-2.35075900	1.84152400	-0.00000400
C	-3.60721400	1.28886100	0.00002800
C	1.17819300	1.04600800	-0.00003400
C	1.35308500	-0.35989700	-0.00004400
C	2.62654000	-0.92634300	-0.00000600
H	2.75106700	-2.00045400	-0.00001000
C	3.73451000	-0.10362500	0.00003900
C	3.60721400	1.28886100	0.00004600
C	2.35075900	1.84152400	0.00001000
H	-2.75106700	-2.00045400	-0.00001100
H	-2.20778400	2.91253700	0.00000000
H	-4.49190700	1.90845000	0.00005700
H	4.49190700	1.90845000	0.00008000
H	2.20778400	2.91253700	0.00001800

N	0.00000000	1.70909200	-0.00005400
S	0.00000000	-1.46137700	-0.00014900
Cl	5.31975100	-0.81355900	0.00009000
Cl	-5.31975100	-0.81355900	0.00007700
Name of species: 3,7-di-Cl-PhtzN⁻			Y=Cl, anion
Cartesian Coordinates			
-1 1			
C	3.67286200	-0.13673800	-0.22423100
C	2.55759800	-0.91981600	0.03769800
C	1.34405500	-0.31036800	0.31369500
C	1.16870700	1.09947400	0.26267900
C	2.34621100	1.84219900	0.00525600
C	3.57403800	1.24707700	-0.22613600
C	-1.16870700	1.09947400	0.26267900
C	-1.34405500	-0.31036800	0.31369500
C	-2.55759800	-0.91981600	0.03769800
H	-2.63981400	-1.99837300	0.05913200
C	-3.67286200	-0.13673800	-0.22423100
C	-3.57403800	1.24707700	-0.22613600
C	-2.34621100	1.84219900	0.00525600
H	2.63981400	-1.99837300	0.05913200
H	2.24361200	2.91871600	-0.01750000
H	4.45072500	1.84928000	-0.42214700
H	-4.45072500	1.84928000	-0.42214700
H	-2.24361200	2.91871600	-0.01750100
N	0.00000000	1.76968100	0.40218500
S	0.00000000	-1.30566700	0.90909800
Cl	5.22286800	-0.90877300	-0.54786400
Cl	-5.22286800	-0.90877300	-0.54786400
Name of species: 3,7-di-CH₃-PhtzNH			Y=CH ₃ , neutral
Cartesian Coordinates			
0 1			
C	-3.64973600	-0.27380500	0.41762400
C	-2.54036000	-1.04994600	0.08468200
C	-1.34526800	-0.46514900	-0.30749100
C	-1.21486200	0.92520700	-0.33121200
C	-2.30828300	1.70509800	0.02845100
C	-3.51361000	1.10988700	0.38000200
C	1.21486800	0.92519200	-0.33121800
C	1.34524800	-0.46515100	-0.30745100
C	2.54031500	-1.04996200	0.08482600
H	2.60771600	-2.13060700	0.11749100
C	3.64969500	-0.27383800	0.41773300
C	3.51359900	1.10987000	0.38004400
C	2.30830200	1.70508400	0.02845300
H	-2.60780300	-2.13059300	0.11725100
H	-2.21616700	2.78421400	0.02604400
H	-4.35568700	1.73652700	0.64400600
H	0.00001100	2.51302700	-0.67403000
H	4.35567400	1.73650100	0.64408400
H	2.21618600	2.78420000	0.02604800
N	0.00000600	1.50748900	-0.72406500

S	-0.00000100	-1.47195400	-0.87401200
C	4.95330700	-0.92723800	0.79503300
H	5.43114800	-1.37485100	-0.07771600
H	5.64287400	-0.19942700	1.21949300
H	4.79617400	-1.71682500	1.52985900
C	-4.95325100	-0.92726300	0.79515800
H	-4.79642500	-1.71418800	1.53292300
H	-5.64417300	-0.19872300	1.21614900
H	-5.42933600	-1.37832900	-0.0767610
Name of species: 3,7-di-CH₃-PhtzNH^{•+}			Y= CH ₃ , radical cation
Cartesian Coordinates			
1 2			
C	-3.77236600	0.27614600	0.00000300
C	-2.63464900	1.05633700	0.00000000
C	-1.35996600	0.47613600	-0.00000200
C	-1.22755400	-0.92340800	-0.00000100
C	-2.38805200	-1.71866800	0.00000200
C	-3.62428800	-1.12887900	0.00000400
C	1.22755400	-0.92340800	-0.00000100
C	1.35996600	0.47613600	-0.00000300
C	2.63464900	1.05633700	-0.00000100
H	2.72075600	2.13551600	-0.00000200
C	3.77236600	0.27614600	0.00000200
C	3.62428800	-1.12887900	0.00000400
C	2.38805200	-1.71866800	0.00000200
H	-2.72075600	2.13551600	-0.00000100
H	-2.29150100	-2.79676100	0.00000300
H	-4.50973100	-1.75070500	0.00000600
H	0.00000000	-2.54043600	-0.00000300
H	4.50973100	-1.75070500	0.00000700
H	2.29150100	-2.79676100	0.00000400
N	0.00000000	-1.53003200	-0.00000200
S	0.00000000	1.55117800	-0.00000900
C	5.14273800	0.88448300	0.00000400
H	5.70018600	0.56225400	0.88012200
H	5.70018500	0.56226000	-0.88011700
H	5.09490600	1.97046200	0.00000700
C	-5.14273800	0.88448300	0.00000600
H	-5.70019100	0.56225100	-0.88010800
H	-5.70018000	0.56226400	0.88013100
H	-5.09490600	1.97046200	-0.00000200
Name of species: 3,7-di-CH₃-PhtzN[•]			Y= CH ₃ , radical
Cartesian Coordinates			
0 2			
C	3.76685700	-0.23810800	0.00008400
C	2.63256600	-1.03076600	-0.00009100
C	1.35487500	-0.46780300	-0.00004600
C	1.17817800	0.93546200	0.00009800
C	2.35601200	1.72489000	0.00041800
C	3.60551700	1.15982700	0.00047200
C	-1.17817800	0.93546200	-0.00007500
C	-1.35487500	-0.46780300	0.00006200

C	-2.63256600	-1.03076500	0.00006800
H	-2.73331500	-2.10958800	0.00015100
C	-3.76685700	-0.23810700	-0.00013500
C	-3.60551700	1.15982700	-0.00053000
C	-2.35601200	1.72489000	-0.00043300
H	2.73331500	-2.10958800	-0.00019400
H	2.21631600	2.79673500	0.00069100
H	4.48351600	1.79351000	0.00079900
H	-4.48351600	1.79351000	-0.00089800
H	-2.21631500	2.79673500	-0.00071400
N	0.00000000	1.60133200	0.00002000
S	0.00000000	-1.56812900	0.00002400
C	-5.14279300	-0.84326900	0.00082100
H	-5.70000700	-0.53153400	0.88540100
H	-5.70662700	-0.51973700	-0.87521500
H	-5.09425300	-1.93041600	-0.00649300
C	5.14279300	-0.84326900	-0.00080300
H	5.70041700	-0.53073500	-0.88483900
H	5.70622200	-0.52053000	0.87579100
H	5.09424900	-1.93042100	0.00552500
Name of species: 3,7-di-CH₃-PhtzN⁻			Y= CH ₃ , anion
Cartesian Coordinates			
-1 1			
C	3.71846900	-0.26047400	0.31723700
C	2.57014900	-1.02687800	0.10628700
C	1.35012900	-0.44408800	-0.19502600
C	1.17043700	0.96565200	-0.23519400
C	2.35123400	1.71589100	-0.02602800
C	3.57775600	1.12412600	0.23044000
C	-1.17081500	0.96607900	-0.23749300
C	-1.34999200	-0.44441400	-0.19529000
C	-2.57004800	-1.02717200	0.10331700
H	-2.63043000	-2.11035800	0.14664800
C	-3.71993700	-0.26068800	0.30931300
C	-3.58057700	1.12298700	0.21535600
C	-2.35316600	1.71549000	-0.03821000
H	2.63079100	-2.10999800	0.14947700
H	2.25004500	2.79289600	-0.06169000
H	4.44727900	1.75532400	0.38331400
H	-4.45199800	1.75369800	0.35855800
H	-2.25428200	2.79240700	-0.08209400
N	0.00007500	1.62667900	-0.41525400
S	0.00021300	-1.48125800	-0.70342600
C	-5.04676400	-0.91340500	0.60288200
H	-5.00483000	-1.52339400	1.50894500
H	-5.81930600	-0.15703600	0.74755800
H	-5.36816000	-1.56412900	-0.21462800
C	5.05130500	-0.91201700	0.58480000
H	5.75864700	-0.18608400	0.98860400
H	4.95788600	-1.72549100	1.30739800
H	5.49135800	-1.33099000	-0.32485100
Name of species: 3,7-di-OCH₃-PhtzNH			Y= OCH ₃ , neutral

Cartesian Coordinates				
0 1				
C	-3.62698000	-0.27157100	0.28969200	
C	-2.52929100	-1.06040500	-0.05288700	
C	-1.34393200	-0.46975500	-0.45048900	
C	-1.21275800	0.92320300	-0.47401600	
C	-2.30146300	1.69640400	-0.10269500	
C	-3.51390400	1.11299500	0.26131700	
C	1.21275500	0.92320500	-0.47401600	
C	1.34393100	-0.46975300	-0.45048900	
C	2.52929200	-1.06040100	-0.05288700	
H	2.62676500	-2.13626900	-0.01377200	
C	3.62698000	-0.27156600	0.28969100	
C	3.51390100	1.11300000	0.26131700	
C	2.30145900	1.69640700	-0.10269600	
H	-2.62676300	-2.13627300	-0.01377100	
H	-2.21282900	2.77566800	-0.10582400	
H	-4.34192600	1.75055500	0.52897900	
H	-0.00000300	2.50648000	-0.84597700	
H	4.34192100	1.75056300	0.52897800	
H	2.21282400	2.77567100	-0.10582400	
N	-0.00000200	1.50072100	-0.89090600	
S	0.00000100	-1.47623000	-1.01891300	
O	-4.75566700	-0.94846200	0.64180600	
O	4.75566700	-0.94845900	0.64180500	
C	-5.88770300	-0.18012200	1.00416700	
H	-6.66969400	-0.89347000	1.24363900	
H	-5.67637700	0.43819900	1.87929400	
H	-6.21192700	0.45254800	0.17516700	
C	5.88770900	-0.18012900	1.00416800	
H	6.66969500	-0.89348300	1.24363800	
H	6.21193800	0.45254100	0.17516900	
H	5.67638900	0.43819200	1.87929600	
Name of species: 3,7-di-OCH₃-PhtzNH^{•+}			Y= OCH ₃ , radical cation	
Cartesian Coordinates				
1 2				
C	-3.76568500	-0.26135700	0.00005100	
C	-2.62685000	-1.06352800	-0.00001600	
C	-1.36509400	-0.49331900	-0.00012900	
C	-1.22829900	0.91146400	-0.00014300	
C	-2.38382800	1.70851600	-0.00006100	
C	-3.63449000	1.14247200	0.00002900	
C	1.22830000	0.91146400	-0.00014300	
C	1.36509400	-0.49331900	-0.00012900	
C	2.62685000	-1.06352800	-0.00001600	
H	2.75530700	-2.13721900	0.00002000	
C	3.76568500	-0.26135700	0.00005100	
C	3.63449000	1.14247200	0.00002900	
C	2.38382800	1.70851600	-0.00006100	
H	-2.75530700	-2.13721900	0.00002000	
H	-2.28162700	2.78622700	-0.00004900	
H	-4.50447900	1.78012800	0.00008300	

H	0.00000000	2.52587100	-0.00026100
H	4.50447900	1.78012800	0.00008300
H	2.28162800	2.78622700	-0.00004900
N	0.00000000	1.51548600	-0.00024000
S	0.00000000	-1.57669600	-0.00029700
O	-4.93185300	-0.90280200	0.00011000
O	4.93185300	-0.90280200	0.00011000
C	-6.14769500	-0.14659400	0.00042000
H	-6.94307800	-0.88213500	0.00062200
H	-6.21166500	0.46795500	0.89785400
H	-6.21213500	0.46796500	-0.89697500
C	6.14769500	-0.14659400	0.00042000
H	6.94307800	-0.88213400	0.00062200
H	6.21213500	0.46796500	-0.89697500
H	6.21166500	0.46795600	0.89785400
Name of species: 3,7-di-OCH₃-PhtzN[•]			Y= OCH ₃ , radical
Cartesian Coordinates			
0 2			
C	3.75569300	-0.23669500	0.00002900
C	2.62524600	-1.04718000	-0.00004000
C	1.35836800	-0.48602300	-0.00004400
C	1.17949600	0.92189800	0.00003100
C	2.35247900	1.70684200	0.00010100
C	3.61636100	1.15706600	0.00010000
C	-1.17949500	0.92189900	0.00003300
C	-1.35836800	-0.48602300	-0.00004000
C	-2.62524600	-1.04717800	-0.00003300
H	-2.76194400	-2.12015800	-0.00008800
C	-3.75569300	-0.23669300	0.00004000
C	-3.61636000	1.15706800	0.00011000
C	-2.35247800	1.70684300	0.00010700
H	2.76194400	-2.12016000	-0.00009700
H	2.21356200	2.77866400	0.00016000
H	4.47866900	1.80551600	0.00016000
H	-4.47866700	1.80551900	0.00017000
H	-2.21356000	2.77866500	0.00016400
N	0.00000100	1.58721800	0.00004800
S	0.00000000	-1.58909100	-0.00019100
O	4.94648300	-0.88365200	0.00002700
O	-4.94648300	-0.88365100	0.00004000
C	6.12747900	-0.09745000	-0.00007000
H	6.95252200	-0.80197200	-0.00016000
H	6.17848900	0.52694800	-0.89364400
H	6.17866200	0.52691700	0.89351400
C	-6.12748100	-0.09745200	0.00000800
H	-6.95252200	-0.80197600	-0.00005400
H	-6.17862500	0.52690200	0.89360500
H	-6.17853500	0.52695800	-0.89355300
Name of species: 3,7-di-OCH₃-PhtzN⁻			Y= OCH ₃ , anion
Cartesian Coordinates			
-1 1			
C	3.73476600	-0.14162000	-0.11543700

C	2.59022500	-0.91386400	-0.27249700
C	1.35337400	-0.30635700	-0.42593400
C	1.18351700	1.10343400	-0.35772300
C	2.38233800	1.84337800	-0.21750100
C	3.62617200	1.24273800	-0.10597300
C	-1.14645900	1.10302800	-0.13823100
C	-1.32806900	-0.30595500	-0.18088200
C	-2.51824800	-0.91342600	0.19085900
H	-2.60680200	-1.99337500	0.17533200
C	-3.61340600	-0.14142900	0.55847000
C	-3.49910000	1.24276100	0.56685400
C	-2.29400300	1.84271700	0.23828200
H	2.67575300	-1.99339900	-0.31529000
H	2.28258800	2.92051300	-0.19395200
H	4.52467300	1.83964400	-0.00685400
H	-4.35569900	1.83988600	0.85603700
H	-2.18309900	2.91852000	0.27010000
N	0.00541300	1.77505300	-0.38768300
S	-0.04172700	-1.29997400	-0.89654400
O	4.98009600	-0.75442700	0.01638900
O	-4.81690600	-0.75430900	0.90549700
C	5.26561900	-1.08780600	1.36304600
H	6.24799900	-1.55820200	1.37906200
H	5.27542300	-0.19059900	1.98841800
H	4.51867300	-1.78207200	1.75732800
C	-5.64600300	-0.97554200	-0.22110600
H	-6.55985600	-1.44795100	0.13721000
H	-5.88818900	-0.02991500	-0.71415700
H	-5.15159100	-1.63128500	-0.94319600
Name of species: 3,7-di-NH₂-PhtzNH			Y= NH ₂ , neutral
Cartesian Coordinates			
0 1			
C	3.63531300	-0.28304800	-0.43806600
C	2.53021800	-1.06463000	-0.10085100
C	1.34429200	-0.47218400	0.30904400
C	1.21173700	0.91530500	0.34820400
C	2.30439200	1.69128800	-0.02195200
C	3.50576400	1.10474800	-0.39317400
C	-1.21173700	0.91530500	0.34820400
C	-1.34429300	-0.47218400	0.30904400
C	-2.53021800	-1.06463000	-0.10085200
H	-2.59262900	-2.14428200	-0.15250300
C	-3.63531300	-0.28304800	-0.43806600
C	-3.50576400	1.10474800	-0.39317400
C	-2.30439200	1.69128800	-0.02195200
H	2.59262900	-2.14428200	-0.15250100
H	2.21856900	2.77088700	-0.00936200
H	4.34402800	1.73072400	-0.67028300
H	0.00000000	2.49662600	0.73046700
H	-4.34402900	1.73072500	-0.67028100
H	-2.21856900	2.77088700	-0.00936200
N	0.00000000	1.49087500	0.77612500

S	0.00000000	-1.48381000	0.87000700
N	4.82288400	-0.88112800	-0.87652300
H	5.64526200	-0.31517800	-0.75132700
H	4.96701400	-1.81902300	-0.54183000
N	-4.82288400	-0.88112900	-0.87652300
H	-4.96701800	-1.81902000	-0.54182200
H	-5.64526000	-0.31517500	-0.75133600
Name of species: 3,7-di-NH₂-PhtzNH^{•+}			Y= NH ₂ , radical cation
Cartesian Coordinates			
1 2			
C	-3.78068400	-0.27068300	0.00005000
C	-2.62956400	-1.06775600	-0.00001800
C	-1.36986500	-0.49347600	-0.00005300
C	-1.22838900	0.90721400	-0.00001100
C	-2.38832600	1.70462800	0.00005800
C	-3.63177000	1.13831700	0.00008600
C	1.22839100	0.90721500	-0.00001200
C	1.36986800	-0.49347300	-0.00004900
C	2.62956400	-1.06775700	-0.00000800
H	2.72460000	-2.14576700	-0.00003200
C	3.78068600	-0.27068500	0.00006200
C	3.63177200	1.13831600	0.00008800
C	2.38832800	1.70462900	0.00005500
H	-2.72460100	-2.14576600	-0.00003800
H	-2.28717300	2.78250000	0.00009100
H	-4.51153900	1.76686600	0.00014500
H	0.00000000	2.52137300	-0.00000300
H	4.51154200	1.76686400	0.00013700
H	2.28717700	2.78250000	0.00008300
N	0.00000100	1.51150800	-0.00003100
S	-0.00000500	-1.57931500	-0.00021400
N	-5.01438700	-0.82300300	0.00011900
H	-5.83802500	-0.25015100	-0.00001600
H	-5.14076200	-1.81833000	-0.00009000
N	5.01438800	-0.82300500	0.00008400
H	5.14076300	-1.81833300	0.00019700
H	5.83802600	-0.25015400	0.00025200
Name of species: 3,7-di-NH₂-PhtzN[•]			Y= NH ₂ , radical
Cartesian Coordinates			
0 2			
C	3.76743100	-0.24205300	0.00388500
C	2.62832600	-1.04269300	-0.00459000
C	1.35987400	-0.47515500	-0.00924600
C	1.17862200	0.92863600	-0.00523600
C	2.35780300	1.71239200	0.00006200
C	3.61148800	1.15606500	0.00186100
C	-1.17862200	0.92863600	-0.00523700
C	-1.35987400	-0.47515600	-0.00924600
C	-2.62832600	-1.04269300	-0.00458900
H	-2.73161900	-2.12117800	-0.01264900
C	-3.76743100	-0.24205300	0.00388500
C	-3.61148800	1.15606500	0.00186000

C	-2.35780300	1.71239200	0.00005900
H	2.73161900	-2.12117800	-0.01265000
H	2.22178000	2.78474200	0.00135000
H	4.48923400	1.78949100	-0.00210100
H	-4.48923400	1.78949100	-0.00210200
H	-2.22178000	2.78474200	0.00134600
N	0.00000000	1.59451800	-0.00462000
S	0.00000000	-1.57862300	-0.02264300
N	5.03377300	-0.80599200	-0.03870600
H	5.78483400	-0.22584300	0.29248500
H	5.10604100	-1.76024400	0.26876400
N	-5.03377100	-0.80599200	-0.03870200
H	-5.10604400	-1.76024300	0.26876900
H	-5.78483900	-0.22583800	0.29246400
Name of species: 3,7-di-NH₂-PhtzN⁻			Y= NH ₂ , anion
Cartesian Coordinates			
-1 1			
C	3.70283500	-0.26999500	0.31659900
C	2.56202600	-1.03714200	0.10172000
C	1.34627400	-0.44399800	-0.21619800
C	1.16907200	0.96232400	-0.24758800
C	2.35402300	1.70585800	-0.03068100
C	3.58166800	1.11493000	0.21858400
C	-1.16907100	0.96232700	-0.24758700
C	-1.34627200	-0.44399600	-0.21619000
C	-2.56202200	-1.03713700	0.10173800
H	-2.61828500	-2.12014000	0.15321100
C	-3.70283600	-0.26999000	0.31659900
C	-3.58167200	1.11493500	0.21855900
C	-2.35402800	1.70586300	-0.03070100
H	2.61829200	-2.12014600	0.15317200
H	2.26003800	2.78322500	-0.07550800
H	4.46380000	1.73228500	0.34553200
H	-4.46381100	1.73228200	0.34548400
H	-2.26004600	2.78322900	-0.07554800
N	-0.00000100	1.62878500	-0.43267600
S	-0.00000100	-1.47638500	-0.74527700
N	4.97726600	-0.86913900	0.58392800
H	5.36691100	-0.52141000	1.44875400
H	4.88898100	-1.87154900	0.66252400
N	-4.97727200	-0.86912100	0.58395800
H	-4.88903900	-1.87155800	0.66226400
H	-5.36675600	-0.52161000	1.44894700
Name of species: 3,7-di-CF₃-PhtzNH			Y= CF ₃ , neutral
Cartesian Coordinates			
0 1			
C	3.62100100	0.02651100	0.17885100
C	2.53234700	-0.70680000	-0.27730100
C	1.33978700	-0.06244700	-0.56471200
C	1.21556600	1.31340700	-0.35025300
C	2.30930400	2.03387900	0.12434000
C	3.51489900	1.39734700	0.37029100

C	-1.21556300	1.31341900	-0.35019700
C	-1.33985400	-0.06242700	-0.56474700
C	-2.53244000	-0.70671400	-0.27736900
H	-2.61262100	-1.77559500	-0.41877700
C	-3.62104100	0.02662900	0.17890200
C	-3.51485900	1.39742300	0.37048000
C	-2.30921400	2.03390100	0.12453700
H	2.61244300	-1.77569300	-0.41864600
H	2.21263900	3.09745400	0.29926400
H	4.36234300	1.96159500	0.73117000
H	0.00000000	2.93829400	-0.41416100
H	-4.36223300	1.96168400	0.73149300
H	-2.21247400	3.09744600	0.29959900
N	0.00000900	1.95112000	-0.61245400
S	-0.00002900	-0.95141200	-1.30834500
C	-4.92883400	-0.66016200	0.40650200
C	4.92882400	-0.66020400	0.40651800
F	-5.68135300	-0.69264000	-0.71218200
F	-4.76651100	-1.93570400	0.79718900
F	-5.66451400	-0.04077200	1.34578000
F	4.76659900	-1.93609600	0.79609500
F	5.66391400	-0.04137400	1.34664500
F	5.68194900	-0.69152600	-0.71178400
Name of speciesL 3,7-di-CF₃-PhtzNH⁺			Y= CF ₃ , radical cation
Cartesian Coordinates			
1 2			
C	-3.74024700	0.02998600	-0.00540800
C	-2.62937800	-0.77271800	-0.00417400
C	-1.35453300	-0.18555000	-0.00210200
C	-1.22727300	1.21590900	-0.00125300
C	-2.38419500	2.01682700	-0.00221300
C	-3.62249600	1.43157900	-0.00402900
C	1.22727200	1.21591400	0.00110200
C	1.35453700	-0.18554800	0.00187800
C	2.62938600	-0.77270900	0.00404700
H	2.73086400	-1.84971100	0.00545300
C	3.74025300	0.02999600	0.00542800
C	3.62249700	1.43158700	0.00412300
C	2.38419400	2.01683200	0.00223100
H	-2.73086000	-1.84971900	-0.00562100
H	-2.28526000	3.09427300	-0.00186300
H	-4.51418100	2.04370000	-0.00550700
H	-0.00000300	2.83315900	-0.00017500
H	4.51417500	2.04371700	0.00572000
H	2.28525500	3.09427800	0.00198000
N	0.00000100	1.82208500	-0.00014100
S	0.00000600	-1.26052400	-0.00023000
C	5.12413700	-0.56514000	-0.00004500
C	-5.12414000	-0.56512900	0.00022100
F	5.82573700	-0.12161500	1.04854600
F	5.08772100	-1.89814400	0.05140000
F	5.78034300	-0.20507600	-1.10888400

F	-5.08775500	-1.89812000	-0.05171100
F	-5.82599700	-0.12123300	-1.04804500
F	-5.78006700	-0.20547100	1.10934600
Name of species: 3,7-di-CF₃-PhtzN[•]			Y= CF ₃ , radical
Cartesian Coordinates			
0 2			
C	-3.73518200	0.05671800	-0.00685300
C	-2.62701600	-0.76147500	-0.01081200
C	-1.35008600	-0.19605800	-0.01012300
C	-1.17711800	1.20995500	-0.00503700
C	-2.34941200	2.01063300	-0.00125600
C	-3.60024900	1.45423900	-0.00169000
C	1.17711800	1.20994300	-0.00494100
C	1.35007100	-0.19606900	-0.01002000
C	2.62699700	-0.76150200	-0.01060100
H	2.74365600	-1.83646300	-0.01481600
C	3.73516700	0.05667900	-0.00646600
C	3.60024900	1.45420600	-0.00130300
C	2.34942200	2.01061200	-0.00101500
H	-2.74368600	-1.83643600	-0.01506100
H	-2.20278600	3.08087200	0.00190100
H	-4.48250600	2.07934600	0.00062800
H	4.48251500	2.07930200	0.00118800
H	2.20280400	3.08085300	0.00217000
N	0.00000400	1.87146100	-0.00340900
S	-0.00001200	-1.29493500	-0.01550200
C	5.11447200	-0.52258900	0.00595600
C	-5.11446900	-0.52258700	0.00598400
F	5.77965500	-0.18317300	1.12610200
F	5.10962900	-1.86198600	-0.06412200
F	5.84789700	-0.06842000	-1.02648800
F	-5.10969500	-1.86181800	-0.06720500
F	-5.84922300	-0.06599900	-1.02442700
F	-5.77822000	-0.18582300	1.12780100
Name of species: 3,7-di-CF₃-PhtzN⁻			Y= CF ₃ , anion
Cartesian Coordinates			
-1 1			
C	3.68991700	0.05068000	0.15017800
C	2.56214900	-0.71980700	-0.14000000
C	1.34606200	-0.11406800	-0.38225700
C	1.16872600	1.29461100	-0.27640100
C	2.34427000	2.03899200	-0.00259500
C	3.56954300	1.44085900	0.19606600
C	-1.16871800	1.29461700	-0.27640900
C	-1.34606100	-0.11406800	-0.38226800
C	-2.56214800	-0.71980400	-0.14002200
H	-2.64049100	-1.79762000	-0.19823200
C	-3.68992200	0.05068200	0.15015000
C	-3.56954300	1.44086000	0.19603500
C	-2.34427100	2.03899500	-0.00262400
H	2.64049400	-1.79762300	-0.19820600
H	2.23037700	3.11230300	0.06189600

H	4.43969300	2.04735300	0.41030500
H	-4.43969400	2.04735600	0.41026600
H	-2.23038500	3.11230700	0.06186500
N	0.00000200	1.96531100	-0.37205500
S	0.00000300	-1.09177600	-0.99888200
C	-5.01194400	-0.58647200	0.31282400
C	5.01194700	-0.58647200	0.31281400
F	-5.74569800	-0.62733100	-0.83646200
F	-4.93195600	-1.87087900	0.72842300
F	-5.80048600	0.06096000	1.20504500
F	4.93196600	-1.87086400	0.72847600
F	5.80052200	0.06099500	1.20498000
F	5.74564200	-0.62737700	-0.83649900
Name of species: 3,7-di-CN-PhtzNH			Y= CN, neutral
Cartesian Coordinates			
0 1			
C	3.63708200	-0.19434700	-0.31007600
C	2.53655800	-0.96716600	0.06351200
C	1.34089000	-0.35257400	0.39225200
C	1.21680700	1.03777800	0.30169700
C	2.31561700	1.80081800	-0.09048400
C	3.52469800	1.19350100	-0.37872200
C	-1.21680700	1.03777800	0.30169700
C	-1.34089000	-0.35257400	0.39225200
C	-2.53655800	-0.96716600	0.06351200
H	-2.62231200	-2.04358600	0.11339300
C	-3.63708200	-0.19434600	-0.31007600
C	-3.52469800	1.19350100	-0.37872200
C	-2.31561700	1.80081800	-0.09048400
H	2.62231100	-2.04358600	0.11339300
H	2.21952800	2.87622900	-0.16455100
H	4.37833800	1.78736100	-0.67097200
H	-4.37833900	1.78736100	-0.67097200
H	-2.21952800	2.87622900	-0.16455100
N	0.00000000	1.64948800	0.60515000
S	0.00000000	-1.30826600	1.04532500
H	0.00000000	2.65140500	0.50506500
C	-4.88062800	-0.83075700	-0.62400100
C	4.88062800	-0.83075700	-0.62400100
N	5.87860900	-1.33947200	-0.87658400
N	-5.87860800	-1.33947200	-0.87658400
Name of species: 3,7-di-CN-PhtzNH⁺			Y= CN, radical cation
Cartesian Coordinates			
1 2			
C	-3.74886500	-0.16740200	0.00001800
C	-2.62717300	-0.97178400	-0.00002500
C	-1.35573700	-0.38815400	-0.00003700
C	-1.22704500	1.01511800	-0.00000400
C	-2.38237000	1.81726300	0.00003900
C	-3.62336900	1.23797000	0.00004800
C	1.22704500	1.01511800	0.00000000
C	1.35573700	-0.38815400	-0.00003500

C	2.62717300	-0.97178400	-0.00002200
H	2.73199900	-2.04846500	-0.00004700
C	3.74886500	-0.16740200	0.00002500
C	3.62336900	1.23797000	0.00005800
C	2.38237000	1.81726300	0.00004700
H	-2.73199900	-2.04846500	-0.00004800
H	-2.28228900	2.89466300	0.00006600
H	-4.51379500	1.84997100	0.00008100
H	4.51379500	1.84997100	0.00009500
H	2.28228900	2.89466300	0.00007600
N	0.00000000	1.61956300	-0.00000800
S	0.00000000	-1.46474600	-0.00011900
H	0.00000000	2.63094800	0.00000600
C	-5.05009800	-0.76247200	0.00003100
N	-6.09501300	-1.23505300	0.00004100
C	5.05009800	-0.76247200	0.00003900
N	6.09501300	-1.23505300	0.00005000
Name of species: 3,7-di-CN-PhtzN[•]			Y= CN, radical
Cartesian Coordinates			
0 2			
C	-3.74249800	-0.13046400	0.00000100
C	-2.62463800	-0.95172300	-0.00000500
C	-1.35106900	-0.39032300	-0.00000400
C	-1.17672400	1.01844300	0.00000200
C	-2.34689700	1.82108900	0.00000800
C	-3.60012000	1.27029600	0.00000700
C	1.17672400	1.01844300	0.00000300
C	1.35106900	-0.39032300	-0.00000400
C	2.62463800	-0.95172300	-0.00000400
H	2.74748400	-2.02636100	-0.00000900
C	3.74249800	-0.13046400	0.00000300
C	3.60012000	1.27029600	0.00000900
C	2.34689700	1.82108900	0.00000900
H	-2.74748400	-2.02636100	-0.00001000
H	-2.19820500	2.89103800	0.00001300
H	-4.48156300	1.89468700	0.00001100
H	4.48156300	1.89468700	0.00001400
H	2.19820500	2.89103800	0.00001400
N	0.00000000	1.67674500	0.00000400
S	0.00000000	-1.48913400	-0.00001500
C	-5.04849800	-0.71460900	0.00000000
N	-6.09895000	-1.17873500	0.00000000
C	5.04849800	-0.71460900	0.00000200
N	6.09895000	-1.17873500	0.00000200
Name of species: 3,7-di-CN-PhtzN⁻			Y= CN, anion
Cartesian Coordinates			
-1 1			
C	3.70612000	-0.16124200	-0.23030200
C	2.56742500	-0.94992300	-0.00453900
C	1.34772700	-0.36323200	0.24925600
C	1.16908100	1.05047700	0.21788800
C	2.34508800	1.81381300	0.00331400

C	3.57467600	1.23445600	-0.20784900
C	-1.16908100	1.05047700	0.21788800
C	-1.34772700	-0.36323200	0.24925600
C	-2.56742500	-0.94992300	-0.00453900
H	-2.65524400	-2.02865000	0.00087200
C	-3.70612000	-0.16124200	-0.23030200
C	-3.57467600	1.23445600	-0.20784900
C	-2.34508800	1.81381300	0.00331400
H	2.65524400	-2.02865000	0.00087200
H	2.22703000	2.88846800	-0.00029500
H	4.44805500	1.85152000	-0.37008900
H	-4.44805500	1.85152000	-0.37008900
H	-2.22703000	2.88846800	-0.00029500
N	0.00000000	1.71301600	0.33629400
S	0.00000000	-1.37935400	0.79406400
C	-4.97184900	-0.76914900	-0.46249100
C	4.97184900	-0.76914900	-0.46249100
N	5.99945500	-1.25760900	-0.65024200
N	-5.99945500	-1.25760900	-0.650242
Name of species: 3,7-di-NO₂-PhtzNH			Y= NO ₂ , neutral
Cartesian Coordinates			
0 1			
C	3.62131000	-0.06390900	-0.21004100
C	2.54007000	-0.85167000	0.15556300
C	1.34132400	-0.23498500	0.46743300
C	1.21792800	1.15576900	0.36141300
C	2.31885100	1.91990300	-0.02589500
C	3.53281100	1.31503200	-0.29892300
C	-1.21788800	1.15577600	0.36141600
C	-1.34129700	-0.23497600	0.46743500
C	-2.54005000	-0.85165400	0.15556900
H	-2.64863900	-1.92462600	0.21189900
C	-3.62129700	-0.06389400	-0.21003700
C	-3.53277300	1.31505000	-0.29891600
C	-2.31880700	1.91991400	-0.02588800
H	2.64865900	-1.92464600	0.21188500
H	2.22001700	2.99408000	-0.11036000
H	4.39758300	1.89066800	-0.59030400
H	-4.39753500	1.89069800	-0.59029600
H	-2.21996300	2.99409100	-0.11034800
N	0.00002300	1.77025900	0.64491100
S	0.00001000	-1.18788300	1.12217400
N	4.89806100	-0.71744900	-0.51520200
N	-4.89808000	-0.71741900	-0.51519800
O	5.82687400	-0.00823300	-0.83075400
O	4.94216600	-1.92401000	-0.43254600
O	-5.82690600	-0.00824000	-0.83077800
O	-4.94231400	-1.92397100	-0.43250600
H	0.00002600	2.77161400	0.53905500
Name of species: 3,7-di-NO₂-PhtzNH^{•+}			Y= NO ₂ , radical cation
Cartesian Coordinates			
1 2			

C	3.72026200	-0.04486700	-0.00076200
C	2.62447300	-0.86457800	0.00033400
C	1.35290500	-0.27631500	0.00135800
C	1.22712400	1.12839500	0.00115400
C	2.38249700	1.93064100	0.00005000
C	3.62540800	1.35097600	-0.00085300
C	-1.22714000	1.12839200	0.00117400
C	-1.35291700	-0.27631700	0.00138300
C	-2.62448000	-0.86458600	0.00038200
H	-2.75479700	-1.93863100	0.00043600
C	-3.72027200	-0.04487700	-0.00070100
C	-3.62542400	1.35096600	-0.00081500
C	-2.38251400	1.93063600	0.00008100
H	2.75479200	-1.93862200	0.00037900
H	2.28265800	3.00794400	-0.00014700
H	4.52827500	1.94382500	-0.00171300
H	-4.52829600	1.94381000	-0.00168200
H	-2.28267900	3.00793900	-0.00012300
N	-0.00000800	1.73369700	0.00202100
S	0.00000100	-1.35201200	0.00396900
N	5.06448600	-0.66823400	-0.00179700
N	-5.06448300	-0.66824600	-0.00175000
O	6.00421500	0.08415700	-0.00232900
O	5.10242600	-1.87231000	-0.00191600
O	-6.00419000	0.08416000	-0.00255500
O	-5.10238400	-1.87231600	-0.00179100
H	-0.00000900	2.74508300	0.00204400
Name of species: 3,7-di-NO₂-PhtzN[•]			Y= NO ₂ , radical
Cartesian Coordinates			
0 2			
C	3.71585200	-0.01515000	0.00001800
C	2.62210400	-0.85173900	-0.00000400
C	1.34885200	-0.28775900	-0.00001200
C	1.17632000	1.12269800	0.00000100
C	2.34622000	1.92735900	0.00002300
C	3.60095600	1.37846900	0.00003000
C	-1.17632500	1.12269600	-0.00000600
C	-1.34885400	-0.28776200	-0.00001800
C	-2.62210600	-0.85174300	-0.00001300
H	-2.76679400	-1.92258900	-0.00001700
C	-3.71585200	-0.01515400	0.00000100
C	-3.60096200	1.37846500	0.00000900
C	-2.34622700	1.92735600	0.00000800
H	2.76679100	-1.92258400	-0.00001200
H	2.19676600	2.99699800	0.00003400
H	4.49250000	1.98596300	0.00004600
H	-4.49250900	1.98595600	0.00001700
H	-2.19677500	2.99699500	0.00001800
N	-0.00000400	1.77993600	-0.00000200
S	-0.00000200	-1.38560600	-0.00005200
N	5.05504600	-0.61781300	0.00002700
N	-5.05504200	-0.61781600	0.00000400
O	6.00129900	0.13571300	-0.00000500

O	5.12521600	-1.82618900	0.00000200
O	-6.00129000	0.13572000	-0.00002100
O	-5.12520200	-1.82619400	0.00006600
Name of species: 3,7-di-NO₂-PhtzN⁻			Y= NO ₂ , anion
Cartesian Coordinates			
-1	1		
C	3.69721800	-0.03627000	-0.14483700
C	2.57578900	-0.84562500	0.06301700
C	1.35049600	-0.26481200	0.28660400
C	1.16978100	1.15084700	0.24308800
C	2.34404900	1.92418600	0.04467600
C	3.57962900	1.35498800	-0.14124000
C	-1.16978000	1.15084600	0.24308500
C	-1.35049500	-0.26481200	0.28660200
C	-2.57578700	-0.84562600	0.06301200
H	-2.69162300	-1.91952600	0.07431300
C	-3.69721700	-0.03627000	-0.14484300
C	-3.57962700	1.35498700	-0.14124600
C	-2.34404800	1.92418600	0.04467300
H	2.69162500	-1.91952500	0.07431700
H	2.21583100	2.99717200	0.03092400
H	4.46058300	1.95861100	-0.29645700
H	-4.46058200	1.95861000	-0.29646300
H	-2.21583100	2.99717100	0.03092100
N	0.00000000	1.81064300	0.33686300
S	0.00000000	-1.28875400	0.80281900
N	4.97714800	-0.64377500	-0.35405800
N	-4.97714700	-0.64377500	-0.35406500
O	5.94638800	0.08217500	-0.52975200
O	5.05206800	-1.86429200	-0.35021700
O	-5.94638900	0.08217800	-0.52974200
O	-5.05207400	-1.86429200	-0.35021000

Table S11. Cartesian coordinates of the all of the reactive complexes (RC), transition state (TS) and post-complexes (PC) of the reaction between 3,7-diY-PhozNHs and HOO[•] optimized at M05-2X/6-311++G(d,p) level of theory in the gas phase (Y = H, F, Cl, CH₃, OCH₃, NH₂, CF₃, CN, NO₂)

3,7-di- H -PhozNH + HOO [•]			
Name of species			RC: 3,7-di- H -PhozN- H.....OOH
0	2		
C	-3.31325300	-1.28822200	0.34239200
C	-2.05526200	-1.87831700	0.44210200
C	-0.95022400	-1.23656900	-0.08062800
C	-1.06908900	0.01123200	-0.70268800
C	-2.32891300	0.60090700	-0.78822200
C	-3.44690500	-0.05214300	-0.27225700
C	1.29869600	0.22521600	-0.62909700
C	1.37368700	-1.02757400	-0.02331500
C	2.54640800	-1.47526800	0.55012400
H	2.55675200	-2.45384000	1.00828100
C	3.67899400	-0.66748100	0.51643400

C	3.61530200	0.58540700	-0.07700600
C	2.42722200	1.03424800	-0.64242300
H	-1.91352200	-2.83965500	0.91528500
H	-2.42629500	1.56380700	-1.27235400
H	-4.41819200	0.41412300	-0.35600500
H	4.48837500	1.22196200	-0.09905100
H	2.36992400	2.01315800	-1.10039500
N	0.08226200	0.61243200	-1.21391600
O	0.27199800	-1.86546700	-0.01905000
H	-0.00751800	1.60288600	-1.38185300
H	-4.17789400	-1.79577500	0.74399700
H	4.60101800	-1.01789400	0.95703400
O	-0.68071000	2.97568900	0.50539400
O	-0.95217800	2.21249700	1.52710000
H	-1.42132400	1.43385100	1.16242400
Name of species		TS: 3,7-di- H -Phoz N...H...OOH	
0 2			
C	-3.78330700	-0.78642900	0.20994300
C	-2.65535400	-1.57810900	0.36989300
C	-1.40582800	-1.04790800	0.09827600
C	-1.26266800	0.26843400	-0.34977000
C	-2.40674300	1.05391300	-0.50522700
C	-3.65666500	0.53244400	-0.22250900
C	1.09252600	-0.01381500	-0.38603600
C	0.92655600	-1.33028500	0.06923500
C	2.01799400	-2.14500700	0.30718800
H	1.84320800	-3.15315100	0.65434700
C	3.29992900	-1.65191200	0.10108200
C	3.48455100	-0.34742700	-0.34950100
C	2.39065900	0.46425400	-0.59806700
H	-2.71919400	-2.60157200	0.71053100
H	-2.28690700	2.07484300	-0.84164600
H	-4.53445300	1.15095000	-0.34148400
H	4.48163800	0.03442200	-0.51473700
H	2.51265300	1.47629700	-0.95427200
N	-0.00782900	0.78178000	-0.64973800
O	-0.31798300	-1.86338600	0.27442900
H	0.11248500	1.84318400	-0.42153300
H	-4.75914200	-1.19710400	0.42541700
H	4.15235200	-2.28876300	0.28929800
O	0.21584300	2.99322900	0.40228900
O	1.53510400	3.08387200	0.74481400
H	1.53853800	2.96980200	1.70293300
Name of species		PC: 3,7-di- H -Phoz N....H-OOH	
0 2			
C	3.87640600	-0.51589100	0.04441900
C	2.86503300	-1.46169300	0.05774400
C	1.54591100	-1.03847800	0.02484200
C	1.20656700	0.32977100	-0.01968100
C	2.25980800	1.26724100	-0.03413800
C	3.57130700	0.85080700	-0.00222200
C	-1.04182500	-0.20525000	-0.03528600

C	-0.72721300	-1.57999800	0.00598600
C	-1.71261800	-2.55361300	0.01731700
H	-1.41931400	-3.59316900	0.04873700
C	-3.04140800	-2.16481300	-0.01194200
C	-3.38468000	-0.80674500	-0.05045700
C	-2.40445700	0.15972600	-0.06070400
H	3.07188900	-2.52164000	0.09192000
H	1.99710400	2.31600600	-0.07084900
H	4.36888600	1.57953700	-0.01407500
H	-4.42534100	-0.51612400	-0.07096800
H	-2.63736900	1.21621500	-0.07819000
N	-0.08294300	0.75739800	-0.05090600
O	0.57239300	-1.99096800	0.03477800
H	-0.49504500	2.52774400	-0.28699900
H	4.90740000	-0.83862100	0.06955400
H	-3.81659800	-2.91754800	-0.00393500
O	-0.74296200	3.47519100	-0.36700400
O	-1.98958800	3.49009800	0.32310100
H	-1.76674100	3.96486000	1.12888600
3,7-di-F-PhozNH + HOO [•]			
Name of species		RC: 3,7-di-F-PhozN–H.....OOH	
0 2			
C	-3.44642700	-0.94011400	0.21235000
C	-2.24995500	-1.63430000	0.22993800
C	-1.11900700	-0.99277100	-0.23620900
C	-1.16631500	0.32210300	-0.70254700
C	-2.38424300	0.98904100	-0.69075900
C	-3.53995400	0.35900400	-0.23772400
C	1.21308400	0.36811800	-0.69435800
C	1.21465100	-0.94751300	-0.23044200
C	2.36670900	-1.54527500	0.24156700
H	2.35039100	-2.56437700	0.59755400
C	3.53395900	-0.80329500	0.23367000
C	3.57813200	0.50019900	-0.21139700
C	2.40156900	1.08472200	-0.66983500
H	-2.19505900	-2.65154300	0.58737300
H	-2.43049000	2.00790500	-1.05198100
H	-4.49463500	0.86291700	-0.23496900
H	4.51110900	1.04310300	-0.19669200
H	2.40785500	2.10709700	-1.02389700
N	0.01362900	0.90355500	-1.18531300
O	0.06136700	-1.70306000	-0.26491500
H	-0.00658500	1.91136100	-1.22020700
O	-0.39571400	3.42938000	0.50192200
O	-0.05861000	2.54084500	1.39567400
H	-0.48687500	2.80872200	2.22540700
F	-4.55744000	-1.56519300	0.65792600
F	4.66625400	-1.38446300	0.68514400
Name of species		TS: 3,7-di-F-PhozN...H...OOH	
0 2			
C	-3.68262000	-0.74762400	0.10495100
C	-2.53230000	-1.48903700	0.28204000

C	-1.31983000	-0.87364700	0.02363700
C	-1.25336600	0.44993900	-0.41947700
C	-2.44348600	1.15949100	-0.58608900
C	-3.66687800	0.56964200	-0.31960600
C	1.11387200	0.30489000	-0.44666800
C	1.02130000	-1.02079500	0.00225600
C	2.15090600	-1.78313300	0.23448000
H	2.06574800	-2.80304200	0.57741600
C	3.38303600	-1.19611200	0.02020800
C	3.52728400	0.10653500	-0.42139600
C	2.38391000	0.85062700	-0.65959600
H	-2.56955300	-2.51366000	0.61979700
H	-2.38758300	2.18598100	-0.92144900
H	-4.59593700	1.10602400	-0.43867200
H	4.51424300	0.51458800	-0.57848000
H	2.45304200	1.86855500	-1.01230500
N	-0.02824900	1.04817100	-0.69861000
O	-0.18881900	-1.62323300	0.21142100
H	0.03428600	2.09509200	-0.39212900
O	0.10053200	3.17818400	0.51855600
O	1.41313100	3.26243300	0.87668800
H	1.41383500	3.07981800	1.82460600
F	-4.86591000	-1.33567800	0.35734200
F	4.48590500	-1.93035300	0.25040700
Name of species		PC: PC: 3,7-di-F-PhozN.....H–OOH	
O 2			
C	3.31144200	-1.46109400	-0.00923000
C	2.06474900	-2.05056400	0.01218500
C	0.96467800	-1.21130900	0.00141900
C	1.09390200	0.19308000	-0.03179600
C	2.39529500	0.73597400	-0.04876700
C	3.50182800	-0.08309200	-0.03857900
C	-1.20592300	0.42183900	-0.02251000
C	-1.35864400	-0.97985000	0.01393100
C	-2.60436400	-1.58279800	0.03915200
H	-2.70291900	-2.65745100	0.06648200
C	-3.71006700	-0.75900200	0.02550800
C	-3.62418400	0.62898000	-0.01209600
C	-2.37546100	1.20864400	-0.03644800
H	1.94743800	-3.12333500	0.03586400
H	2.48817500	1.81379800	-0.05778500
H	4.50595500	0.31327600	-0.05117900
H	-4.52965200	1.21712600	-0.02241300
H	-2.25737600	2.28315100	-0.06629700
N	0.01446900	1.01975700	-0.04725400
O	-0.26741200	-1.79394300	0.02307700
H	0.20056400	2.82906300	-0.30405000
O	0.34685500	3.79573500	-0.39249100
O	1.55625900	3.95269700	0.34461300
H	1.25538700	4.42609500	1.12543100
F	4.39177600	-2.25742100	0.00031000
F	-4.92666200	-1.32488800	0.04930300

3,7-di-Cl-PhozNH + HOO [•]			
Name of species		RC: 3,7-di-Cl-PhozN...H...OOH	
0 2			
C	-3.46026300	-0.76108900	0.06518300
C	-2.25414100	-1.44762100	0.00683000
C	-1.12321200	-0.77017900	-0.40149200
C	-1.16727200	0.58380900	-0.73811600
C	-2.38438500	1.24878700	-0.66337600
C	-3.53754200	0.57966000	-0.26752800
C	1.21105400	0.62322100	-0.72900400
C	1.21070100	-0.73204200	-0.39760500
C	2.36170400	-1.37377600	0.01221300
H	2.32711200	-2.42354300	0.26283300
C	3.54259600	-0.64642700	0.08183000
C	3.57487600	0.69931800	-0.23853900
C	2.40181400	1.33071800	-0.63604400
H	-2.18516700	-2.49422300	0.26334600
H	-2.43040900	2.29745600	-0.92573400
H	-4.48416600	1.09649900	-0.21848800
H	4.50202000	1.24885800	-0.17554500
H	2.41206100	2.38365900	-0.88559900
N	0.01309600	1.20666200	-1.15546600
O	0.05518700	-1.47763100	-0.50783100
H	-0.00739400	2.21446900	-1.11493100
O	-0.55327500	3.65922700	0.58902100
O	0.00506200	2.84325300	1.44060200
H	-0.39467400	3.03163700	2.30579700
Cl	-4.89430900	-1.60984600	0.57560200
Cl	5.00357800	-1.44936000	0.59122900
Name of species		TS: 3,7-di-Cl-PhozN...H...OOH	
0 2			
C	-3.65374800	-0.62811800	0.02109500
C	-2.47508500	-1.34254900	0.15932400
C	-1.27574900	-0.68914800	-0.06129600
C	-1.23664300	0.65747400	-0.43290400
C	-2.44215500	1.34889200	-0.56393900
C	-3.65003900	0.71630500	-0.33331700
C	1.13053800	0.57075600	-0.44997700
C	1.06842400	-0.77835700	-0.07100200
C	2.21503900	-1.52110200	0.13580400
H	2.13512400	-2.55823200	0.42473400
C	3.44573900	-0.90381400	-0.03008800
C	3.54563400	0.43002000	-0.40451800
C	2.38855600	1.15851800	-0.61916100
H	-2.47222000	-2.38491200	0.44133500
H	-2.41037300	2.39380200	-0.84135700
H	-4.58285600	1.25084500	-0.42914400
H	4.51668300	0.88375200	-0.53367000
H	2.43726700	2.19495300	-0.91806400
N	-0.02676900	1.29168700	-0.67927200
O	-0.12823600	-1.42177300	0.08925800
H	0.00430800	2.34492700	-0.36449000

O	0.00883900	3.42648600	0.52380000
O	1.31486100	3.59280600	0.88564700
H	1.31644800	3.44597000	1.83948100
Cl	4.89174500	-1.83195100	0.22900900
Cl	-5.16726100	-1.43312600	0.30312800
Name of species		PC: PC: 3,7-di- Cl -PhozN.....H-OOH	
0 2			
C	3.40616200	-1.08438800	-0.00905100
C	2.17280100	-1.71216100	0.00601100
C	1.03819600	-0.92074100	-0.00650000
C	1.10726000	0.48781200	-0.03550900
C	2.38552600	1.08262900	-0.04719200
C	3.52290300	0.30879800	-0.03497300
C	-1.19777600	0.62005000	-0.02994800
C	-1.29242700	-0.78669100	0.00205800
C	-2.51227000	-1.44057900	0.02481500
H	-2.54569500	-2.51943800	0.04953200
C	-3.66518000	-0.67563900	0.01363100
C	-3.62104800	0.72140600	-0.02045900
C	-2.40023600	1.35525700	-0.04215700
H	2.08166900	-2.78774000	0.02738200
H	2.43631400	2.16337200	-0.05363700
H	4.50295600	0.76139100	-0.04326700
H	-4.54199200	1.28474600	-0.02981300
H	-2.33083400	2.43427300	-0.06843100
N	-0.00478800	1.26785700	-0.05077800
O	-0.16838900	-1.55454200	0.00969800
H	0.10533400	3.09018500	-0.29680700
O	0.21291900	4.06194800	-0.38041200
O	1.42288900	4.26143300	0.34549000
H	1.11261600	4.72332600	1.12947700
Cl	4.84232800	-2.05381500	0.00938600
Cl	-5.20642600	-1.47032300	0.04464100
3,7-di-CH ₃ -PhozNH + HOO [•]			
Name of species		RC: 3,7-di- CH₃ -PhozN... H ...OOH	
0 2			
C	-3.53804800	-0.90221700	0.21392700
C	-2.31953000	-1.58478000	0.19046600
C	-1.17292300	-0.96017700	-0.25290300
C	-1.19136700	0.36976200	-0.67700200
C	-2.39536000	1.05702700	-0.63719700
C	-3.55635900	0.42302400	-0.20228000
C	1.18865300	0.36716600	-0.67776700
C	1.16736600	-0.96271100	-0.25329300
C	2.31278900	-1.58971500	0.18975800
H	2.24013400	-2.62138600	0.50875000
C	3.53296400	-0.91004900	0.21238300
C	3.55423000	0.41492200	-0.20451500
C	2.39441500	1.05149000	-0.63904900
H	-2.24912100	-2.61670100	0.50915800
H	-2.42279900	2.09017400	-0.95988000
H	-4.48727300	0.97449300	-0.18921700

H	4.48653400	0.96406300	-0.19258700
H	2.42433900	2.08424000	-0.96288400
N	-0.00080000	0.94206500	-1.14034000
O	-0.00349800	-1.69286300	-0.30566400
H	0.00007500	1.95023200	-1.16160800
O	0.01715100	3.61024200	0.43618500
O	0.00681800	2.68673800	1.35712700
H	0.04987100	3.14748200	2.21106900
C	-4.79102600	-1.60268800	0.66987600
H	-5.61739200	-0.89919700	0.75645500
H	-5.08267700	-2.38044200	-0.03758000
H	-4.64366000	-2.07625500	1.64099300
C	4.78439600	-1.61336600	0.66821400
H	4.63683100	-2.08444100	1.64052400
H	5.07272500	-2.39353500	-0.03793000
H	5.61303500	-0.91224400	0.75222900
Name of species			TS: 3,7-di-NH ₂ -PhozN...H...OOH
0 2			
C	-3.71526500	-0.77592100	0.10877700
C	-2.52510600	-1.48210700	0.24730400
C	-1.31137800	-0.86655000	-0.00425300
C	-1.24784400	0.46670700	-0.41372600
C	-2.44251100	1.17534800	-0.54797500
C	-3.65464900	0.56373200	-0.28399500
C	1.12098100	0.33479300	-0.43560700
C	1.03496300	-1.00244600	-0.02010200
C	2.17107700	-1.75364000	0.20611900
H	2.05121300	-2.78090300	0.52368400
C	3.43616700	-1.19408900	0.03224100
C	3.52767700	0.13604400	-0.37575800
C	2.39013500	0.89053900	-0.61431400
H	-2.51898200	-2.51740700	0.56146300
H	-2.39428400	2.21338500	-0.84900700
H	-4.57071200	1.13040600	-0.38411900
H	4.50175600	0.58519000	-0.51591600
H	2.46100500	1.91878900	-0.93695100
N	-0.02553400	1.06839200	-0.68858100
O	-0.17575100	-1.61908900	0.15790700
H	0.02644500	2.11642700	-0.42895700
O	0.05653800	3.24764000	0.47781600
O	1.36389400	3.38989300	0.83973000
H	1.36836300	3.21372500	1.78852900
C	-5.03845300	-1.44934600	0.35359500
H	-5.43712300	-1.86099000	-0.57557300
H	-4.93598000	-2.26715100	1.06507000
H	-5.76775200	-0.74122300	0.74446400
C	4.66827200	-2.02687900	0.26026800
H	4.60365700	-2.56936500	1.20334400
H	4.78954200	-2.76137700	-0.53768100
H	5.55974000	-1.40291400	0.28265100
Name of species			PC: 3,7-di-CH ₃ -PhozN.....H-OOH
0 2			

C	-3.74085600	-0.80116400	0.02257400
C	-2.58808600	-1.57249100	0.03854600
C	-1.34371900	-0.96178500	0.01482300
C	-1.20325100	0.43862100	-0.02429100
C	-2.38667300	1.20644100	-0.04125000
C	-3.61980000	0.59986100	-0.01767100
C	1.09636500	0.23307400	-0.03284100
C	0.98389200	-1.17027900	0.00393800
C	2.09796500	-1.99446500	0.01640100
H	1.94976500	-3.06538200	0.04367200
C	3.36924300	-1.43944600	-0.00656100
C	3.49936900	-0.03885800	-0.03842800
C	2.39653700	0.78114700	-0.05119000
H	-2.63328100	-2.65271000	0.06736000
H	-2.28545600	2.28312500	-0.07328300
H	-4.51651700	1.20585000	-0.03163400
H	4.48994200	0.39660400	-0.05198300
H	2.48427600	1.85959900	-0.06322700
N	0.00995800	1.05011800	-0.04953400
O	-0.24346600	-1.76630400	0.02773500
H	0.17191100	2.84656500	-0.29799500
O	0.29181300	3.81926200	-0.38681700
O	1.49986500	4.01236100	0.34412000
H	1.18543100	4.45443600	1.13756700
C	-5.10128900	-1.43980900	0.04921300
H	-5.68264100	-1.14201600	-0.82428200
H	-5.02609300	-2.52516500	0.05719600
H	-5.65461700	-1.12772800	0.93600700
C	4.59403400	-2.31066300	-0.00324100
H	4.33019500	-3.36060000	0.10483500
H	5.15040700	-2.19130300	-0.93410400
H	5.25889400	-2.03575300	0.81616200
3,7-di-OCH ₃ -PhozNH + HOO [•]			
Name of species		RC: 3,7-di-OCH ₃ -PhozN...H...OOH	
O 2			
C	-3.41284500	-0.82528300	0.07430000
C	-2.18326900	-1.48961700	0.06087000
C	-1.05895000	-0.84299600	-0.39699100
C	-1.11004300	0.48686800	-0.84137100
C	-2.33443200	1.13805400	-0.80918100
C	-3.49018700	0.49215900	-0.35775100
C	1.26646000	0.54500100	-0.80480200
C	1.27325000	-0.78366900	-0.37480000
C	2.41607000	-1.38403100	0.09900900
H	2.39376100	-2.41282900	0.42666800
C	3.60603300	-0.65645300	0.14764400
C	3.62282500	0.66973800	-0.26550200
C	2.44775300	1.25992300	-0.73211800
H	-2.11638800	-2.51226400	0.40151600
H	-2.39273200	2.16315800	-1.15084500
H	-4.42313800	1.03279100	-0.35844300
H	4.52537100	1.25895000	-0.23100000

H	2.45995200	2.29397600	-1.05159400
N	0.06770000	1.08238700	-1.31283000
O	0.12108300	-1.54424300	-0.44540600
H	0.03787400	2.09073000	-1.30827500
O	-0.49377000	3.19217700	0.79083500
O	-0.80013100	2.28700000	1.67790100
H	-1.26299500	1.57688000	1.18550500
O	-4.46557600	-1.55219500	0.53269400
O	4.68902800	-1.33395800	0.61775400
C	-5.73467200	-0.92251100	0.54957600
H	-6.42932300	-1.66155100	0.93504300
H	-5.72803600	-0.04964600	1.20548400
H	-6.03553800	-0.62671000	-0.45731600
C	5.91993300	-0.63632100	0.67187300
H	5.85226100	0.22423600	1.34056000
H	6.64650600	-1.34227600	1.06110600
H	6.22589100	-0.30757200	-0.32337100
Name of species		TS: ,7-di-NH ₂ -PhozN...H...OOH	
0 2			
C	-3.67023900	-0.75025300	0.07452200
C	-2.46526300	-1.43406200	0.22385300
C	-1.27802900	-0.78844400	-0.04450700
C	-1.25187900	0.54105200	-0.48184400
C	-2.46370800	1.20598600	-0.62528800
C	-3.67094700	0.57895700	-0.34739000
C	1.12106500	0.47541500	-0.48957800
C	1.07082900	-0.85781100	-0.04888900
C	2.21897800	-1.57262600	0.20416600
H	2.15735900	-2.59832300	0.53579200
C	3.46328100	-0.96476400	0.03153000
C	3.54262800	0.35879600	-0.39775200
C	2.37359900	1.06217100	-0.65692200
H	-2.46110300	-2.46138300	0.55655600
H	-2.44919900	2.23720300	-0.95179100
H	-4.58971400	1.13068800	-0.46449900
H	4.49262100	0.84925600	-0.53743400
H	2.41967200	2.08719300	-0.99429400
N	-0.04378900	1.17168500	-0.77338900
O	-0.12231100	-1.50835300	0.12164700
H	-0.01033900	2.20640300	-0.50676300
O	0.03371600	3.32322200	0.47951300
O	1.28314000	3.30601100	1.01665600
H	1.14965700	3.01936300	1.92878100
O	-4.78866800	-1.46230800	0.36453100
O	4.53730600	-1.74642400	0.30382500
C	-6.03814800	-0.80525400	0.23493500
H	-6.20299100	-0.48228800	-0.79455100
H	-6.78913300	-1.53787300	0.51160400
H	-6.09800500	0.05280300	0.90697000
C	5.82540300	-1.18557200	0.11135100
H	6.53116600	-1.96968000	0.36455000
H	5.96677100	-0.88593800	-0.92847000

H	5.97887900	-0.32794600	0.76877600
Name of species		PC: 3,7-di- OCH₃ -PhozN.....H-OOH	
0 2			
C	-3.67703000	-0.83781900	0.01781500
C	-2.49248300	-1.57300000	0.03311800
C	-1.28718700	-0.90869400	0.00973000
C	-1.20877500	0.50212100	-0.02797500
C	-2.42131200	1.21028500	-0.04441600
C	-3.64090400	0.56268000	-0.02178300
C	1.09859900	0.39916100	-0.03340700
C	1.05019100	-1.01322100	0.00159600
C	2.18982800	-1.78371400	0.01595500
H	2.12475800	-2.86123000	0.04106600
C	3.43481100	-1.15609800	-0.00304800
C	3.52326800	0.24249800	-0.03443200
C	2.36891000	0.99954400	-0.04889300
H	-2.52363500	-2.65198500	0.06127900
H	-2.37044700	2.29042100	-0.07510500
H	-4.54935800	1.14374900	-0.03616400
H	4.48012200	0.73948200	-0.04678000
H	2.40950200	2.08065900	-0.06023700
N	-0.02326600	1.16688200	-0.05121600
O	-0.15073800	-1.66221500	0.02162300
H	0.06040700	2.95926000	-0.29749000
O	0.14091500	3.93714900	-0.38675200
O	1.33999100	4.17962000	0.34464300
H	1.00767100	4.60936300	1.13760300
O	-4.81624200	-1.56586200	0.04415400
O	4.50424700	-1.98315000	0.01269300
C	-6.05352900	-0.86964500	0.02746600
H	-6.82265000	-1.63404300	0.05683700
H	-6.14573200	-0.22218800	0.90083100
H	-6.15467600	-0.28119900	-0.88574300
C	5.79927300	-1.40121000	-0.00722800
H	5.95572600	-0.77221900	0.87038200
H	6.49572600	-2.23268800	0.01078100
H	5.94810300	-0.81722700	-0.91663700
3,7-di-NH ₂ -PhozNH + HOO•			
Name of species		RC: 3,7-di-NH ₂ -PhozN...H...OOH	
0 2			
C	-3.39407700	-0.97047400	0.14743700
C	-2.14461300	-1.59708300	0.16917600
C	-1.02642900	-0.93896000	-0.30193700
C	-1.09733800	0.36797000	-0.79412500
C	-2.34137200	0.99054000	-0.80094800
C	-3.47743300	0.33431700	-0.33618900
C	1.27474000	0.47337000	-0.73968700
C	1.30410200	-0.83330900	-0.26162800
C	2.45672600	-1.40047600	0.24275900
H	2.41545400	-2.41645300	0.61119800
C	3.64122000	-0.66220000	0.27331300
C	3.62085400	0.65267000	-0.19024300

C	2.44897400	1.20981400	-0.68472100
H	-2.02633900	-2.60209400	0.55095800
H	-2.41979100	2.00083900	-1.18065800
H	-4.43116700	0.84406600	-0.35101500
H	4.52385100	1.24762000	-0.15755800
H	2.44774800	2.23153300	-1.04213800
N	0.07199600	0.97693900	-1.27946300
O	0.16717400	-1.62122900	-0.30538300
H	0.02172200	1.98480500	-1.26981400
O	-0.56190000	3.09907700	0.80600400
O	-0.85655600	2.19923900	1.70229100
H	-1.27682900	1.46143200	1.21248200
N	4.80370500	-1.21571600	0.81929600
H	4.85682800	-2.21903900	0.76660600
H	5.65728600	-0.78194600	0.51057800
N	-4.51609700	-1.62111700	0.66309400
H	-5.39778600	-1.27939800	0.31997200
H	-4.47006900	-2.62587800	0.64638000
Name of species		TS: 3,7-di-NH ₂ -PhozN...H...OOH	
0 2			
C	-3.72661800	-0.75171400	0.10986500
C	-2.53130300	-1.45096800	0.27476100
C	-1.32565600	-0.83399000	-0.00123700
C	-1.26313500	0.47998200	-0.46502600
C	-2.46340100	1.16804100	-0.63034100
C	-3.67720500	0.57078900	-0.34520900
C	1.10907600	0.34118900	-0.49280800
C	1.02126300	-0.97632200	-0.02560400
C	2.14838800	-1.73499900	0.21719700
H	2.02183700	-2.75137100	0.56402600
C	3.41777400	-1.19001000	0.01054100
C	3.52145600	0.12468700	-0.45544500
C	2.38407800	0.87032200	-0.70579200
H	-2.52016100	-2.47604300	0.61936400
H	-2.42613100	2.19045300	-0.98205700
H	-4.59615800	1.12428400	-0.48297100
H	4.49743300	0.55626900	-0.63221500
H	2.46454700	1.88333400	-1.07186100
N	-0.03740400	1.07830800	-0.76382700
O	-0.18963900	-1.58185500	0.19185000
H	0.02477300	2.09508000	-0.49115500
O	0.14844300	3.18507300	0.60967600
O	1.44518300	3.13313700	1.00290300
H	1.41626800	2.76072000	1.89349900
N	-4.94805400	-1.37766700	0.34154100
N	4.55393200	-1.96456500	0.21008100
H	-4.92115500	-2.16424700	0.96729200
H	-5.71868000	-0.76013100	0.53099800
H	4.44972200	-2.74773600	0.83151500
H	5.40819300	-1.45603500	0.35813500
Name of species		PC: 3,7-di-NH ₂ -PhozN.....H-OOH	
0 2			

C	3.36469700	-1.45269000	-0.01162000
C	2.08420300	-2.00875900	0.00950500
C	0.98304500	-1.17799500	-0.00428000
C	1.09643200	0.22700500	-0.04200800
C	2.39971400	0.76338800	-0.06166500
C	3.50507100	-0.05248300	-0.04975100
C	-1.20227500	0.43803500	-0.03262700
C	-1.34853100	-0.96364200	0.00763600
C	-2.58417600	-1.57737900	0.03521800
H	-2.63143100	-2.65750300	0.05843300
C	-3.74237200	-0.79785400	0.02332300
C	-3.62500000	0.60361700	-0.02264500
C	-2.38673200	1.20011000	-0.04830800
H	1.93301600	-3.07925700	0.03019800
H	2.49546800	1.84112500	-0.07548700
H	4.49682800	0.37916300	-0.07192200
H	-4.52054500	1.21051100	-0.04274100
H	-2.28874400	2.27707100	-0.08203000
N	0.01260500	1.04709200	-0.05809900
O	-0.24801500	-1.77204600	0.01967000
H	0.17988000	2.82191500	-0.29799300
O	0.30196700	3.79779500	-0.38019600
O	1.50223100	3.98628100	0.36491800
H	1.17760800	4.40851600	1.16493200
N	-4.99022600	-1.39403900	0.00510000
H	-5.04329000	-2.34220600	0.33318600
H	-5.76400400	-0.82193000	0.29419300
N	4.48219700	-2.26557900	-0.04317200
H	5.35213900	-1.84424700	0.23069000
H	4.36713100	-3.20982800	0.27993800
3,7-di-CF ₃ -PhozNH + HOO•			
Name of species		RC: 3,7-di-CF ₃ -PhozN-H.....OOH	
0 2			
C	-3.62170000	-0.40207200	0.00855800
C	-2.43918000	-1.11181700	-0.20058900
C	-1.25753400	-0.42271600	-0.33867900
C	-1.22385000	0.97455200	-0.25725900
C	-2.40795200	1.66568400	-0.03603400
C	-3.61015300	0.97943200	0.09170200
C	1.16406600	0.88079000	-0.25808400
C	1.08861000	-0.51495900	-0.34055500
C	2.21291400	-1.29452000	-0.20495400
H	2.12063200	-2.36921400	-0.27891200
C	3.44711800	-0.67932400	0.00456000
C	3.54272100	0.69855200	0.09114400
C	2.39804100	1.47732700	-0.03436900
H	-2.43115800	-2.19050000	-0.27227600
H	-2.38482100	2.74552700	0.02606700
H	-4.52954900	1.52110200	0.25377200
H	4.50158100	1.16681900	0.25410300
H	2.45916500	2.55550800	0.02909500
N	-0.00296200	1.61594300	-0.41663800

O	-0.11101700	-1.13839100	-0.60763200
H	0.03553600	2.60416200	-0.21648200
O	0.14369200	4.67529200	0.18749200
O	1.39948400	5.02631400	0.15251800
H	1.42256300	5.98252700	0.32461100
C	-4.88821500	-1.17613900	0.16874600
C	4.65117900	-1.54831900	0.15907400
F	-4.89800300	-1.89348000	1.31131200
F	-5.06302100	-2.06176100	-0.83140500
F	-5.97198900	-0.38391200	0.19431900
F	4.75758600	-2.43951700	-0.84557800
F	4.60946600	-2.26960300	1.29829500
F	5.79186300	-0.83973500	0.18615600
Name of species		TS: 3,7-di-CF ₃ -PhozN...H...OOH	
0 2			
C	-3.62371800	-0.37106100	-0.08915400
C	-2.43389000	-1.07461600	0.01291800
C	-1.24166900	-0.39873300	-0.17134400
C	-1.22146400	0.96770200	-0.47007000
C	-2.43452900	1.65592000	-0.56557500
C	-3.63041800	0.99417400	-0.36981900
C	1.14205300	0.91661800	-0.49033900
C	1.10170700	-0.45166200	-0.17805700
C	2.26191300	-1.17895500	0.00221300
H	2.19482000	-2.23087800	0.23774800
C	3.48380900	-0.53425800	-0.12799200
C	3.55399600	0.82024200	-0.44152700
C	2.38886000	1.53933400	-0.62980500
H	-2.41351400	-2.13179600	0.23329500
H	-2.41125200	2.71340500	-0.79006900
H	-4.56733300	1.52601900	-0.44503800
H	4.51450800	1.30159700	-0.55116700
H	2.41528700	2.58834100	-0.88325800
N	-0.02354800	1.62794200	-0.68486600
O	-0.08452000	-1.12024600	-0.06237400
H	-0.00974800	2.69420600	-0.31576000
O	-0.03811100	3.71783000	0.54883700
O	1.26382100	3.91723900	0.92220400
H	1.25411200	3.79130100	1.87881400
C	-4.91996700	-1.07271000	0.17405500
C	4.74682100	-1.29504500	0.13387300
F	-4.83638100	-2.39121300	-0.06382700
F	-5.91367300	-0.58576000	-0.58712100
F	-5.30840100	-0.93037700	1.45602600
F	5.13969200	-1.17129800	1.41680500
F	5.76214700	-0.85407100	-0.62597900
F	4.60299400	-2.60817900	-0.10435900
Name of species		PC: 3,7-di-CF ₃ -PhozN.....H-OOH	
0 23			
C	-3.62093500	-0.43845800	-0.00497600
C	-2.44986500	-1.17078200	-0.00204600
C	-1.24437000	-0.48584300	-0.01958400

C	-1.18840600	0.92262600	-0.03745200
C	-2.40880700	1.63276800	-0.04137100
C	-3.60728000	0.96425200	-0.02450900
C	1.11871500	0.85223900	-0.04590100
C	1.08660500	-0.55776600	-0.03175000
C	2.24543200	-1.31623800	-0.03154000
H	2.17898000	-2.39409300	-0.02598600
C	3.46059500	-0.65685100	-0.04550900
C	3.53286500	0.74322200	-0.05444300
C	2.37873800	1.48814100	-0.05501300
H	-2.45023900	-2.25047100	0.01090800
H	-2.36310000	2.71300200	-0.05743700
H	-4.54089000	1.50877400	-0.02847500
H	4.49745900	1.22960200	-0.06601700
H	2.39512900	2.56973700	-0.05248400
N	-0.01388000	1.60076400	-0.05306400
O	-0.10151100	-1.22184200	-0.02199300
H	0.04974600	3.44705100	-0.28590600
O	0.13960500	4.41864600	-0.36719300
O	1.35203100	4.63596400	0.34947000
H	1.04307300	5.11163000	1.12588100
C	-4.94976500	-1.12902100	0.03026300
C	4.73434900	-1.44379600	0.01103600
F	5.25118800	-1.44890500	1.25407500
F	4.55493100	-2.72393400	-0.34682400
F	5.67267600	-0.92427200	-0.79670500
F	-4.83460400	-2.46203000	-0.03818500
F	-5.73167400	-0.73701500	-0.99073800
F	-5.61932000	-0.84047700	1.16120800
3,7-di-CN-PhozNH + HOO•			
Name of species		RC: 3,7-di-CN-PhozN...H...OOH	
O 2			
C	3.69433600	-0.71876300	-0.09705800
C	2.53486000	-1.47938400	0.08693300
C	1.32782300	-0.83970900	0.24343000
C	1.23869900	0.55614400	0.20520900
C	2.39655200	1.30242400	0.01152500
C	3.62220400	0.67114700	-0.13215600
C	-1.14355300	0.36917100	0.20650900
C	-1.01398500	-1.02355600	0.24536200
C	-2.10710400	-1.84352900	0.09173600
H	-1.97303400	-2.91470700	0.12595300
C	-3.37132900	-1.27293200	-0.09115600
C	-3.51595500	0.11120900	-0.12913200
C	-2.40330000	0.92614600	0.01146200
H	2.56949400	-2.55839400	0.11967100
H	2.32993900	2.38180900	-0.01832100
H	4.52163700	1.25109600	-0.27552700
H	-4.49489000	0.54451500	-0.27154500
H	-2.50594200	2.00258400	-0.01901400
N	-0.00575600	1.14394900	0.37134200
O	0.21024400	-1.60951200	0.48387300

H	-0.08384500	2.13809600	0.21524000
O	-0.26734400	4.19606700	-0.14223800
O	-1.52890000	4.52446400	-0.10732600
H	-1.56851000	5.48186800	-0.27055100
C	4.95773100	-1.37441300	-0.24891300
C	-4.51754000	-2.11766700	-0.23641500
N	5.97351100	-1.89624900	-0.37276400
N	-5.43967900	-2.79237700	-0.35349100
Name of species:			TS: 3,7-di-CN-PhozN...H...OOH
O 2			
C	-3.66841100	-0.68985200	0.03061900
C	-2.48513800	-1.41454700	0.15205400
C	-1.28240000	-0.76919600	-0.05411000
C	-1.23474800	0.58813900	-0.39546100
C	-2.43375900	1.29873400	-0.51200200
C	-3.64247500	0.67059200	-0.29609200
C	1.12593100	0.48983400	-0.41870900
C	1.06035800	-0.86906000	-0.06612300
C	2.20469300	-1.61341600	0.12862200
H	2.12163700	-2.65524900	0.40026300
C	3.44591100	-0.99652100	-0.02355000
C	3.53580600	0.35256600	-0.37864100
C	2.38389000	1.08578600	-0.58061700
H	-2.48886000	-2.46308100	0.41118000
H	-2.38878600	2.34884400	-0.76595100
H	-4.56938900	1.21757700	-0.38092500
H	4.50594200	0.81087200	-0.49973000
H	2.42892600	2.12760400	-0.86001900
N	-0.02536900	1.21530600	-0.62741000
O	-0.13887400	-1.50802600	0.07842700
H	0.00965500	2.30438200	-0.31448200
O	-0.00621200	3.37890600	0.47055000
O	1.29647300	3.58827800	0.83653200
H	1.27292200	3.56921500	1.80097000
C	-4.92274400	-1.34609600	0.24815500
C	4.64115800	-1.75765800	0.18337500
N	-5.93030000	-1.86840000	0.42235500
N	5.60258700	-2.36251700	0.35069900
Name of species			PC: 3,7-di-CN-PhozN.....H–OOH
O 2			
C	-3.69315100	-0.71348000	0.01499400
C	-2.53984800	-1.49007400	0.02355100
C	-1.31332800	-0.85319000	0.00565600
C	-1.20395500	0.55478400	-0.01907800
C	-2.39609800	1.31074100	-0.02904500
C	-3.62092200	0.69159200	-0.01186000
C	1.09798600	0.39921400	-0.02390100
C	1.01450400	-1.01086400	-0.00283500
C	2.14160600	-1.80962400	0.00362200
H	2.03853100	-2.88454200	0.01819500
C	3.38901700	-1.19535600	-0.00908100
C	3.50754900	0.20672200	-0.02612900

C	2.38019700	0.98988800	-0.03262000
H	-2.58391500	-2.56897800	0.04257000
H	-2.30881200	2.38836300	-0.04975400
H	-4.53321200	1.26931400	-0.01923900
H	4.48991000	0.65466100	-0.03270400
H	2.43560100	2.07028700	-0.03227100
N	-0.00583800	1.18613600	-0.03514100
O	-0.19764500	-1.62967100	0.01018300
H	0.13102100	3.03523700	-0.29616900
O	0.26949700	3.99799100	-0.39823800
O	1.47832300	4.17134400	0.33628600
H	1.18617600	4.71001400	1.07732200
C	-4.97269900	-1.35446500	0.03495500
C	4.56965800	-2.00544700	-0.00192500
N	-6.00119900	-1.86448700	0.05206100
N	5.51849600	-2.65226600	0.00427700
3,7-di-NO ₂ -PhozNH + HOO [•]			
Name of species		RC: 3,7-di- NO ₂ -PhozN- H.....OOH	
0 2			
C	3.63457400	-0.56992800	-0.05144300
C	2.47478900	-1.31914600	0.11427400
C	1.28254900	-0.64887700	0.25039100
C	1.23079400	0.75037100	0.20616700
C	2.40869400	1.47052200	0.02909200
C	3.62235300	0.81231900	-0.09457300
C	-1.15739800	0.62794800	0.20936800
C	-1.06582000	-0.76943100	0.25302200
C	-2.18330000	-1.55822400	0.11811500
H	-2.10317200	-2.63376900	0.15208500
C	-3.41389300	-0.93142300	-0.04532200
C	-3.54281500	0.44474500	-0.08775700
C	-2.40293100	1.22422900	0.03381000
H	2.50562700	-2.39718300	0.14877700
H	2.36702500	2.55076700	-0.00452400
H	4.54616700	1.35283700	-0.22641800
H	-4.51771700	0.88767200	-0.21744500
H	-2.47193100	2.30302800	0.00107700
N	0.00195200	1.37010500	0.34935100
O	0.14348000	-1.38959800	0.47507200
H	-0.04874100	2.36913200	0.21212100
O	-0.16343700	4.42342400	-0.12260900
O	-1.42179500	4.76419400	-0.09626500
H	-1.45128600	5.72275000	-0.25551000
N	-4.61080300	-1.76364400	-0.17696900
N	4.91018600	-1.27579300	-0.18348500
O	5.90901900	-0.60629300	-0.33221500
O	4.88870700	-2.48567600	-0.13657900
O	-5.67281000	-1.19962600	-0.32510600
O	-4.46577600	-2.96499400	-0.13021300
Name of species		TS: 3,7-di- NO ₂ -PhozN- H...OOH	
0 2			
C	-3.62027500	-0.51379900	-0.02792100

C	-2.45127800	-1.24514700	0.08589500
C	-1.25599400	-0.57959400	-0.10020400
C	-1.22447700	0.78768400	-0.40822100
C	-2.43064500	1.48927600	-0.51370400
C	-3.63510900	0.84489100	-0.31828000
C	1.13544400	0.71887700	-0.42911900
C	1.08627300	-0.65012600	-0.10867200
C	2.23930600	-1.38517800	0.07137800
H	2.19242500	-2.43394700	0.32059600
C	3.45121500	-0.72968700	-0.07019100
C	3.54891000	0.61675900	-0.39267800
C	2.38511900	1.33701600	-0.57778000
H	-2.46723800	-2.29818700	0.32128800
H	-2.39552600	2.54522900	-0.74288600
H	-4.57605200	1.36674500	-0.39077900
H	4.52046800	1.07278500	-0.49933400
H	2.41503700	2.38522700	-0.83361100
N	-0.02331100	1.43559100	-0.61822300
O	-0.10446500	-1.30564700	0.01927000
H	-0.00290700	2.52632100	-0.26208600
O	-0.03548800	3.55517500	0.54368200
O	1.26647700	3.77606100	0.90872600
H	1.24584900	3.74031800	1.87280100
N	-4.89861700	-1.21066700	0.17762400
N	4.68620200	-1.50331000	0.12826600
O	-4.85461500	-2.39254200	0.43120000
O	-5.91036200	-0.55526700	0.07998300
O	4.57101500	-2.67391600	0.41037600
O	5.73582800	-0.91656800	-0.00107300
Name of species		PC: 3,7-di- NO ₂ -PhozN.....H-OOH	
0 2			
C	-3.63266500	-0.55310500	0.00850900
C	-2.48747900	-1.32379200	0.01558200
C	-1.27396600	-0.66043900	0.00135200
C	-1.19470100	0.75069600	-0.01788300
C	-2.40086300	1.48482900	-0.02549000
C	-3.61526900	0.84367000	-0.01218300
C	1.10998000	0.64274600	-0.02175800
C	1.05466600	-0.76992300	-0.00535300
C	2.19811900	-1.54652300	0.00061300
H	2.14140200	-2.62403200	0.01209100
C	3.41083800	-0.88636900	-0.00893700
C	3.52504300	0.50570300	-0.02202200
C	2.37863900	1.26274500	-0.02820700
H	-2.53378200	-2.40184100	0.03017900
H	-2.33424900	2.56380200	-0.04167100
H	-4.54691700	1.38693500	-0.01752900
H	4.50417100	0.95766700	-0.02605900
H	2.41021300	2.34390900	-0.02524000
N	-0.01000100	1.40595700	-0.03134700
O	-0.14344900	-1.41244300	0.00424000
H	0.08953000	3.26705400	-0.29187500

O	0.21419300	4.23044900	-0.39674500
O	1.42310500	4.42126200	0.33350300
H	1.12930000	4.97209600	1.06491400
N	4.63903100	-1.69856900	-0.00102300
N	-4.93208900	-1.24373400	0.02422100
O	-5.92509900	-0.55437100	0.02370800
O	-4.91927500	-2.45292100	0.03692500
O	5.69350000	-1.10741900	-0.00578100
O	4.51048500	-2.90113200	0.01001300

Table S12. Cartesian coordinates of the all of the reactive complexes (RC), transition state (TS) and post-complexes (PC) of the reaction between 3,7-diY-PhtzNHs and HOO[•] optimized at M05-2X/6-311++G(d,p) level of theory in the gas phase (Y= H, F, Cl, CH₃, OCH₃, NH₂, CF₃, CN, NO₂)

3,7-di- H -PhtzNH + HOO•			
Name of species		RC: 3,7-di- H -PhtzN– HOOH	
0 2			
C	3.84749800	0.11286700	-0.58120300
C	3.05204100	-0.99176000	-0.30183600
C	1.73860400	-0.82313500	0.11623200
C	1.18990800	0.45778900	0.21292300
C	1.98482800	1.56129700	-0.09265700
C	3.30982300	1.38896700	-0.46873800
C	-1.12140800	-0.28504800	0.21725600
C	-0.82118700	-1.64585400	0.11968300
C	-1.79128500	-2.54856100	-0.29476200
H	-1.53161900	-3.59468100	-0.38472600
C	-3.08231000	-2.11439800	-0.57049200
C	-3.38850800	-0.76399900	-0.45682900
C	-2.41102900	0.14894300	-0.08535600
H	3.45048500	-1.99340000	-0.39137600
H	1.55736800	2.55360000	-0.02408800
H	3.91732200	2.25598200	-0.68850900
H	-4.38827000	-0.41388100	-0.67288300
H	-2.64233400	1.20442200	-0.01835800
N	-0.13812000	0.62480500	0.62064900
H	-0.44659300	1.58535600	0.62190300
O	-0.94948200	3.69466600	0.30727500
O	-2.19433100	3.87711800	-0.03824300
H	-2.28640000	4.82287000	-0.24015100
S	0.77556600	-2.21882100	0.63605200
H	4.87438800	-0.02490500	-0.88731000
H	-3.83789600	-2.82478000	-0.87346900
Name of species		TS: 3,7-di- H -PhtzN... H ...OOH	
0 2			
C	-3.90919600	-0.47472400	0.12193700
C	-2.88071000	-1.39285000	0.24019300
C	-1.55648600	-1.00352600	0.04760900
C	-1.25758500	0.32671600	-0.27548600
C	-2.31101200	1.24672400	-0.39240300

C	-3.61829800	0.85258600	-0.19328700
C	1.16860400	0.04703400	-0.29725700
C	1.15643100	-1.31827400	0.03383600
C	2.35634000	-2.00202600	0.20983200
H	2.33009200	-3.05317200	0.46617400
C	3.56918100	-1.34952200	0.06183800
C	3.59024200	0.00331900	-0.27155200
C	2.40698300	0.69163300	-0.45460300
H	-3.09525700	-2.42395300	0.48939100
H	-2.06844000	2.27343100	-0.63164200
H	-4.41461500	1.57746700	-0.28391600
H	4.53180800	0.51905700	-0.39460500
H	2.40877300	1.74092700	-0.71206900
N	0.02518200	0.78869600	-0.50316900
H	0.12826000	1.86032800	-0.36412100
H	-4.93096200	-0.78997000	0.27626900
H	4.49187400	-1.89372700	0.20255700
O	0.10064200	3.13762500	0.30868900
O	1.39332900	3.51785800	0.56242900
H	1.40811800	3.66373600	1.51537300
S	-0.32529100	-2.25008700	0.18786800
Name of species		PC: 3,7-di-H-PhtzN.....H-OOH	
0 2			
C	-3.94129500	-0.30496600	0.03780500
C	-2.99002200	-1.30522600	0.05331600
C	-1.63047100	-0.98714500	0.02298200
C	-1.20558800	0.36249100	-0.02069200
C	-2.20992100	1.36201900	-0.03789900
C	-3.54379100	1.03856300	-0.00967000
C	1.12759600	-0.07466700	-0.03323600
C	1.03274500	-1.48693700	0.00008400
C	2.18316500	-2.27836500	0.00635800
H	2.08546000	-3.35595400	0.03035200
C	3.43210700	-1.69037800	-0.01799200
C	3.54888700	-0.29360000	-0.04613800
C	2.42495100	0.49496100	-0.05316000
H	-3.29038100	-2.34449400	0.08815000
H	-1.88262200	2.39236300	-0.07368300
H	-4.28789500	1.82210700	-0.02447200
H	4.52682800	0.16585700	-0.06142800
H	2.49174100	1.57460900	-0.06093100
N	0.08119400	0.78702800	-0.04871400
H	0.36832100	2.56629900	-0.29886100
H	-4.99061800	-0.56216200	0.06123700
H	4.31671100	-2.31129000	-0.01354100
O	0.48943400	3.53919600	-0.39859600
O	1.68372100	3.75122200	0.34900600
H	1.35412200	4.19983600	1.13269900
S	-0.50096500	-2.31251300	0.03422700
3,7-di-F-PhtzNH + HOO•			
Name of species		RC: 3,7-di-H-PhtzN-H.....OOH	
0 2			

C	3.69940000	-0.60749100	-0.43994100
C	2.69414400	-1.50582400	-0.14191900
C	1.46475900	-1.01262400	0.27598600
C	1.23709900	0.36366300	0.34915200
C	2.26763500	1.23910400	0.01465400
C	3.51415400	0.75764700	-0.36368400
C	-1.17991100	0.19169800	0.35598500
C	-1.21117800	-1.20300900	0.28589000
C	-2.35977200	-1.86584000	-0.12706200
H	-2.38785800	-2.94327700	-0.20507500
C	-3.48382900	-1.11965000	-0.41993700
C	-3.49245900	0.25824500	-0.34824800
C	-2.32480500	0.91201100	0.02293400
H	2.87506100	-2.56817500	-0.22099600
H	2.09203100	2.30576800	0.06330200
H	4.32722800	1.42399100	-0.61092300
H	-4.39254400	0.80250100	-0.59302200
H	-2.30247300	1.99305800	0.06447700
N	-0.01052000	0.84486900	0.76902100
H	-0.08092800	1.85124100	0.75597900
O	-0.05660800	3.99818500	0.30279000
O	-1.17443500	4.40121000	-0.23518100
H	-1.02672800	5.31825300	-0.52037400
S	0.20184500	-2.13020800	0.82020500
F	4.90302500	-1.08579000	-0.82367800
F	-4.60999500	-1.76497200	-0.79449200
Name of species		TS: 3,7-di-F-PhozN...H...OOH	
O 2			
C	-3.82266800	-0.51279900	0.10890200
C	-2.76098900	-1.38129800	0.22214000
C	-1.47372200	-0.90832400	-0.02414200
C	-1.26908200	0.42909900	-0.38499800
C	-2.38074100	1.27831100	-0.48251100
C	-3.65848400	0.81888500	-0.23648200
C	1.16557800	0.31272300	-0.41458700
C	1.24496300	-1.03667900	-0.03011600
C	2.48200100	-1.62711600	0.20502400
H	2.56256700	-2.66237600	0.50525200
C	3.62355300	-0.87040600	0.04733500
C	3.58813600	0.45720100	-0.34074200
C	2.35747600	1.03934500	-0.57142000
H	-2.93649800	-2.41036600	0.50268000
H	-2.21307800	2.31414200	-0.74352200
H	-4.51907300	1.46741200	-0.30454600
H	4.50830100	1.00964800	-0.45661900
H	2.29142500	2.07364600	-0.87399200
N	-0.02290200	0.96609600	-0.67124300
H	0.03342400	2.04122100	-0.49537300
O	0.02666400	3.26976300	0.22864400
O	1.20065500	3.37538100	0.92349800
H	0.92867800	3.35216100	1.84879200
S	-0.16575200	-2.07860900	0.07953900

F	-5.06290800	-0.97529400	0.34893000
F	4.81423200	-1.45195300	0.27727500
Name of species		PC: 3,7-di-F-PhtzN.....H-OOH	
0 2			
C	-3.82761800	-0.57782100	0.02171200
C	-2.78973900	-1.47910800	0.03562600
C	-1.48236900	-0.99470000	0.01259600
C	-1.22180900	0.39633300	-0.02156600
C	-2.33746600	1.26992600	-0.03661800
C	-3.62740900	0.79907600	-0.01532200
C	1.14743200	0.24213600	-0.02735800
C	1.22121500	-1.17114200	-0.00084400
C	2.45280200	-1.82417300	0.00741900
H	2.52182700	-2.90295300	0.02636600
C	3.59958200	-1.06646200	-0.00953800
C	3.58241200	0.32524300	-0.03115200
C	2.36663400	0.96435600	-0.03946000
H	-2.99956500	-2.53929900	0.06280300
H	-2.13748100	2.33221200	-0.06457400
H	-4.47949500	1.46243600	-0.02706800
H	4.51427500	0.87082700	-0.03977900
H	2.30467200	2.04429300	-0.04259400
N	0.00498400	0.97285800	-0.04274600
H	0.07270400	2.77739100	-0.29428600
O	0.08322500	3.75609900	-0.39758700
O	1.25774900	4.09895100	0.33292700
H	0.89331100	4.54120800	1.10485000
S	-0.20317300	-2.17905000	0.02083900
F	-5.08615400	-1.04560400	0.04454400
F	4.78569300	-1.69591800	-0.00183500
3,7-di-Cl-PhtzNH + HOO[•]			
Name of species		RC: 3,7-di-Cl-PhtzN-H..... OOH	
0 2			
C	-3.66450100	-0.58871300	0.29326700
C	-2.60338200	-1.42655600	-0.01388900
C	-1.39652100	-0.87389300	-0.41923700
C	-1.23177500	0.51229000	-0.47233600
C	-2.30538800	1.33376200	-0.13596000
C	-3.52801900	0.78855300	0.22879800
C	1.19165600	0.44948200	-0.48089800
C	1.28609700	-0.94316000	-0.43148900
C	2.46524100	-1.55785600	-0.03316200
H	2.52540500	-2.63523500	0.02577000
C	3.56921100	-0.77568100	0.26902700
C	3.50170000	0.60696400	0.20951400
C	2.30672300	1.21482700	-0.14724700
H	-2.71941900	-2.49928300	0.04586500
H	-2.18138000	2.40828000	-0.17152400
H	-4.36435100	1.42606800	0.47516900
H	4.37005200	1.20041200	0.45507200
H	2.23702300	2.29449600	-0.17178800
N	-0.00661400	1.05852800	-0.86851200

H	0.01895400	2.06689600	-0.84064600
O	-0.12025700	4.18148500	-0.29916900
O	0.81688600	4.49959100	0.55050000
H	0.59668200	5.38574200	0.88249200
Cl	5.05944700	-1.54642700	0.74423700
Cl	-5.18934600	-1.28446600	0.77407300
S	-0.08422800	-1.92628800	-0.97756700
Name of species		TS: 3,7-di-Cl-PhozN...H...OOH	
0 2			
C	-3.81366800	-0.43770600	0.03884600
C	-2.72130100	-1.27873900	0.12988600
C	-1.44234800	-0.77515800	-0.09448300
C	-1.26148400	0.57657900	-0.41377600
C	-2.39059300	1.40437400	-0.49536600
C	-3.65808400	0.91035200	-0.27063400
C	1.17194600	0.50847000	-0.43473900
C	1.27831800	-0.85128100	-0.09573500
C	2.52652300	-1.42391400	0.12162000
H	2.60856400	-2.46847000	0.38766600
C	3.66673000	-0.64993800	-0.00451500
C	3.58890600	0.69464400	-0.34916000
C	2.35010000	1.26221800	-0.56377700
H	-2.86032500	-2.32120700	0.37982600
H	-2.24448000	2.45095400	-0.72484700
H	-4.52238000	1.55503000	-0.32898900
H	4.49013500	1.28113600	-0.44583200
H	2.26651900	2.30563200	-0.82877600
N	-0.02656700	1.14564800	-0.67149200
H	0.00891000	2.22502600	-0.47776200
O	-0.02944400	3.44531100	0.22991900
O	1.12626000	3.57251100	0.95383100
H	0.82828400	3.57258100	1.87115900
Cl	5.21914100	-1.37505900	0.27482800
Cl	-5.40344900	-1.07470400	0.32937300
S	-0.11255200	-1.92226400	-0.01765000
Name of species		PC: 3,7-di-Cl-PhtzN.....H-OOH	
0 2			
C	-3.81157100	-0.51592400	0.01168100
C	-2.73305400	-1.37586800	0.02601200
C	-1.44014400	-0.85417200	0.00631900
C	-1.21929600	0.54366200	-0.02598400
C	-2.36157900	1.38222900	-0.04160800
C	-3.63499900	0.87129200	-0.02334200
C	1.15034300	0.45829200	-0.02871100
C	1.26627100	-0.95227400	-0.00314200
C	2.51654500	-1.56886700	0.00630400
H	2.59758400	-2.64696500	0.02498100
C	3.65454700	-0.78943000	-0.00848700
C	3.58047600	0.60729400	-0.02984700
C	2.34920800	1.21342200	-0.03917600
H	-2.89355000	-2.44478400	0.05115100
H	-2.19518000	2.45049300	-0.06762000

H	-4.49717300	1.52162200	-0.03596700
H	4.48816700	1.19235000	-0.03732300
H	2.25886900	2.29148900	-0.04154700
N	-0.01132000	1.15482000	-0.04452200
H	0.00864300	2.96545200	-0.29438800
O	-0.00604300	3.94371600	-0.39661400
O	1.15591100	4.31660600	0.33916100
H	0.77669500	4.74826200	1.11002800
Cl	-5.41812400	-1.16957100	0.03650400
Cl	5.21087200	-1.55690000	0.00426900
S	-0.12756000	-2.00076000	0.01679300
3,7-di-CH ₃ -PhtzNH + HOO•			
Name of species		RC: 3,7-di-CH ₃ -PhtzN-H..... OOH	
0 2			
C	-3.70848700	-0.67602700	0.42648100
C	-2.62621800	-1.52598900	0.20108200
C	-1.41292700	-1.03804700	-0.26032000
C	-1.23359600	0.33284100	-0.46455200
C	-2.30168200	1.18918100	-0.21631800
C	-3.52636600	0.68478300	0.20484400
C	1.19156400	0.24606000	-0.47268700
C	1.27569500	-1.13340800	-0.27218100
C	2.45485600	-1.70673600	0.18190900
H	2.48502300	-2.77612100	0.35152800
C	3.59432400	-0.93510800	0.40172400
C	3.50438500	0.43720800	0.18927500
C	2.31646900	1.02675700	-0.22380000
H	-2.73144400	-2.59058300	0.37190000
H	-2.17220200	2.25339500	-0.36760500
H	-4.34864700	1.36762000	0.37566500
H	4.37147900	1.06128200	0.36385000
H	2.25741500	2.09925100	-0.35930700
N	-0.00373000	0.82163300	-0.92316700
H	0.03249100	1.82744200	-0.98865800
O	-0.11470600	3.94045700	-0.28823300
O	0.80884600	4.22833800	0.58705000
H	0.46720500	4.97246600	1.10962300
S	-0.10853800	-2.15559600	-0.70100800
C	4.88440200	-1.58029700	0.83577700
H	4.70377000	-2.35244900	1.58326300
H	5.38938900	-2.04837400	-0.01105400
H	5.56205200	-0.84307400	1.26378800
C	-5.02872000	-1.23072400	0.89401600
H	-5.44758200	-1.91640000	0.15629000
H	-4.91307800	-1.77927900	1.82944400
H	-5.74846100	-0.43037800	1.05754700
Name of species		TS: 3,7-di-CH ₃ -PhtzN...H...OOH	
0 2			
C	-3.86223800	-0.53827500	0.12151600
C	-2.75738100	-1.37072200	0.20481900
C	-1.46874100	-0.89833300	-0.04417600
C	-1.26725700	0.44164900	-0.38770700

C	-2.38558800	1.28529000	-0.46268400
C	-3.65283000	0.80494900	-0.21353100
C	1.16731000	0.33447900	-0.41626400
C	1.25371700	-1.01721600	-0.05241900
C	2.49689900	-1.59945600	0.18094300
H	2.53996600	-2.64385700	0.46506200
C	3.67279100	-0.87253300	0.05576800
C	3.58244100	0.47196200	-0.31844100
C	2.35980800	1.06529200	-0.54973800
H	-2.88909700	-2.41176700	0.47309300
H	-2.22564400	2.32716400	-0.70533900
H	-4.49837000	1.47797700	-0.27329900
H	4.48615600	1.05738500	-0.42673700
H	2.29437200	2.10591200	-0.83181200
N	-0.02371500	0.98145400	-0.67653300
H	0.02902400	2.04964100	-0.53785100
O	0.02199000	3.32836700	0.17370800
O	1.15834800	3.43205100	0.92908700
H	0.83710600	3.41750600	1.83821300
S	-0.15534400	-2.06656700	0.02800600
C	-5.25067400	-1.05568500	0.38138800
C	5.01066200	-1.50511100	0.32425600
H	5.47191200	-1.06649500	1.21033400
H	4.91289700	-2.57658500	0.48803000
H	5.68873800	-1.34647900	-0.51456200
H	-5.22528600	-2.08374100	0.73775200
H	-5.84952400	-1.02671700	-0.53013100
H	-5.75696300	-0.44613700	1.13013800
Name of species		PC: 3,7-di-CH ₃ -PhtzN.....H-OOH	
0 2			
C	-3.86695300	-0.61486800	0.02118500
C	-2.78008200	-1.46997200	0.03845600
C	-1.47228900	-0.97952800	0.01300900
C	-1.22025500	0.41043400	-0.02813100
C	-2.34939800	1.26769400	-0.04799200
C	-3.62707300	0.77136700	-0.02418000
C	1.14767000	0.27496900	-0.03197700
C	1.23512300	-1.13513200	-0.00041200
C	2.47633600	-1.77502300	0.00896800
H	2.51086200	-2.85759600	0.03103200
C	3.65464500	-1.05093800	-0.00986600
C	3.57723100	0.35441200	-0.03521800
C	2.36673500	0.99838800	-0.04571100
H	-2.94025300	-2.54086700	0.07086400
H	-2.16317900	2.33267800	-0.08229100
H	-4.46774100	1.45306700	-0.04090300
H	4.49146900	0.93403500	-0.04564200
H	2.30223400	2.07834800	-0.05156900
N	0.00082700	0.99812100	-0.05157000
H	0.06067700	2.78724500	-0.31204700
O	0.06459900	3.76817500	-0.41788400
O	1.19512900	4.13107500	0.37012100

H	0.78341900	4.52707100	1.14331800
S	-0.18248400	-2.15207800	0.02622100
C	-5.27482700	-1.14001400	0.04897700
H	-5.28873200	-2.22777900	0.07457100
H	-5.80577300	-0.76946800	0.92684200
H	-5.82530400	-0.81059500	-0.83319400
C	4.99258800	-1.73495700	-0.00075800
H	5.57067500	-1.45830000	-0.88346700
H	5.56904100	-1.43897900	0.87684200
H	4.88203500	-2.81744100	0.01110200
3,7-di- OCH₃ -PhtzNH + HOO [•]			
Name of species		RC: 3,7-di-OCH₃-PhtzN–H..... OOH	
O 2			
C	-3.57565200	-0.53160400	0.26589000
C	-2.46859600	-1.38136000	0.22078700
C	-1.29065900	-0.96674600	-0.37185600
C	-1.17492800	0.32766800	-0.90215500
C	-2.27666000	1.17280500	-0.83098300
C	-3.48030300	0.74854200	-0.26463100
C	1.24369200	0.34961900	-0.89236600
C	1.38806000	-0.94281000	-0.38032200
C	2.57127300	-1.33941900	0.21656700
H	2.67888800	-2.33164300	0.63182100
C	3.65099400	-0.46023500	0.28172800
C	3.52110600	0.82767600	-0.22569400
C	2.31305900	1.22621400	-0.79217000
H	-2.55455700	-2.37120900	0.64686500
H	-2.19987900	2.17535000	-1.23181400
H	-4.31525700	1.43099200	-0.24322500
H	4.33288800	1.53597100	-0.17508900
H	2.20514500	2.23927100	-1.15797600
N	0.02942800	0.73360400	-1.49848300
H	0.02050900	1.70693800	-1.76183000
O	-0.15792100	3.23176600	0.27687200
O	-0.35918500	2.45367800	1.30291600
H	-0.87360000	1.69073300	0.96541000
S	0.05632100	-2.10015700	-0.56048300
O	-4.69003300	-1.04512900	0.85110200
O	4.77826400	-0.95025300	0.86681100
C	-5.82832000	-0.20555900	0.93553500
H	-6.59507300	-0.79101500	1.43202800
H	-5.61028300	0.68762600	1.52455600
H	-6.17468800	0.08244700	-0.05893500
C	5.88624700	-0.07572000	0.98092300
H	5.63305200	0.79732200	1.58594900
H	6.66742300	-0.64560500	1.47348400
H	6.23343200	0.24518000	-0.00326200
Name of species		TS: 3,7-di-OCH₃-PhtzN...H...OOH	
O 2			
C	3.68081600	-0.74290800	0.05491000
C	2.52238300	-1.50658800	0.18321200
C	1.28030300	-0.95236000	-0.06988800

C	1.16865100	0.39781900	-0.45055200
C	2.34372200	1.14553900	-0.57876100
C	3.58957900	0.59292900	-0.33166700
C	-1.27150200	0.45622700	-0.42851100
C	-1.44727600	-0.88821300	-0.07067900
C	-2.71536400	-1.38495200	0.18696000
H	-2.85855800	-2.41999200	0.46513000
C	-3.83197100	-0.56073100	0.09376600
C	-3.67241700	0.78135600	-0.25228000
C	-2.40242500	1.27054000	-0.50701200
H	2.61730100	-2.54217200	0.47943700
H	2.26290500	2.18127800	-0.87364400
H	4.46779200	1.20916100	-0.44098200
H	-4.51644500	1.44937000	-0.32095800
H	-2.26615300	2.31328400	-0.76012200
N	-0.03593200	1.01627500	-0.72615600
H	-0.00657200	2.07437300	-0.58895900
O	-0.03358500	3.34590300	0.20578300
O	1.12238900	3.44307700	0.92633600
H	0.83974700	3.34022200	1.84290300
S	-0.10926300	-2.03151100	-0.00154200
O	-5.02595400	-1.14767700	0.36153800
O	4.84369400	-1.38631700	0.32384300
C	-6.19118600	-0.34758400	0.24921000
H	-6.30121200	0.03848100	-0.76569800
H	-7.02452300	-1.00185000	0.48298500
H	-6.16545800	0.48008200	0.96030100
C	6.04839400	-0.64977600	0.18906100
H	6.84781400	-1.33988800	0.43745000
H	6.17436400	-0.29561900	-0.83548100
H	6.06613700	0.19584300	0.87878200
Name of species		PC: 3,7-di-OCH ₃ -PhtzN.....H-OOH	
0 2			
C	-3.82936800	-0.65786400	0.01530800
C	-2.72213400	-1.49885000	0.04380300
C	-1.43996100	-0.97353400	0.02335300
C	-1.22558400	0.42716500	-0.02363200
C	-2.37380000	1.24750500	-0.05156100
C	-3.65081900	0.73104400	-0.03384400
C	1.14752100	0.35914100	-0.02558100
C	1.27772300	-1.05222200	0.01280800
C	2.52609600	-1.65280800	0.02144700
H	2.62903000	-2.72920700	0.04770200
C	3.68037600	-0.87726100	-0.00637600
C	3.58386600	0.52062900	-0.03766400
C	2.34065100	1.11356500	-0.04610600
H	-2.88766300	-2.56706900	0.07873900
H	-2.21784600	2.31722500	-0.08847700
H	-4.49440900	1.40283800	-0.05837000
H	4.46541800	1.14235700	-0.05387400
H	2.24492700	2.19108900	-0.05561900
N	-0.02014100	1.04867400	-0.04613200

H	-0.00841700	2.82751200	-0.30706900
O	-0.03071800	3.80963600	-0.41287900
O	1.08390500	4.20317000	0.38340400
H	0.65618500	4.58079000	1.15702400
S	-0.11356100	-2.11218100	0.05149000
O	-5.03603100	-1.26977300	0.03748400
O	4.84890900	-1.55878300	0.00186400
C	-6.19677500	-0.45385400	-0.01646800
H	-7.03907600	-1.13723500	-0.00047500
H	-6.24621600	0.20887700	0.84891000
H	-6.21644200	0.13176100	-0.93679500
C	6.05511600	-0.81074900	-0.04756100
H	6.14583400	-0.16268600	0.82544200
H	6.85639800	-1.54198700	-0.04406600
H	6.10428000	-0.21551700	-0.96052900
3,7-di-NH ₂ -PhtzNH + HOO•			
Name of species		RC: 3,7-di-NH ₂ -PhtzN-H..... OOH	
0 2			
C	-3.66917600	-0.42631700	0.40564500
C	-2.58909700	-1.30538500	0.33749800
C	-1.40165000	-0.91648200	-0.26778100
C	-1.24543000	0.36768000	-0.78371100
C	-2.31146100	1.25509200	-0.67846500
C	-3.51151600	0.86218400	-0.10731900
C	1.17155100	0.32270100	-0.80325000
C	1.27835300	-0.96542600	-0.26900400
C	2.45611100	-1.39406700	0.32554500
H	2.49924300	-2.38635300	0.75627800
C	3.57978000	-0.56558400	0.36568400
C	3.47836500	0.71650700	-0.17383900
C	2.28779600	1.15627100	-0.73875100
H	-2.67072600	-2.30053200	0.75593700
H	-2.19786700	2.26707600	-1.04597900
H	-4.32740100	1.56953500	-0.03792100
H	4.33033600	1.38268900	-0.14049400
H	2.22129500	2.15938200	-1.13992500
N	-0.03115100	0.74006900	-1.40029500
H	-0.01392700	1.71661800	-1.65119100
O	0.19471400	3.19240000	0.42884500
O	0.38370300	2.39801500	1.44441800
H	0.86647700	1.62081000	1.09308300
S	-0.08078900	-2.08728000	-0.44847700
N	-4.85714200	-0.80616200	1.03818500
H	-5.67043800	-0.29081400	0.74649400
H	-5.03029800	-1.79716500	1.05009300
N	4.75282000	-0.99114700	0.99194900
H	4.87604500	-1.98875000	1.03219400
H	5.58911500	-0.52170100	0.68857300
Name of species		TS: 3,7-di-NH ₂ -PhtzN...H...OOH	
0 2			
C	3.66044600	-0.80848000	0.16386000
C	2.49113600	-1.56758700	0.21150800

C	1.26463100	-1.00566500	-0.11181400
C	1.17070700	0.34375000	-0.48252700
C	2.35170900	1.09956100	-0.51959500
C	3.57103100	0.53863400	-0.20745100
C	-1.25740900	0.43087700	-0.46000900
C	-1.44699000	-0.90837300	-0.10593400
C	-2.70907000	-1.38298100	0.23168900
H	-2.82515800	-2.42167200	0.51527000
C	-3.81687800	-0.53949300	0.21860500
C	-3.62815100	0.80503200	-0.12571000
C	-2.37453400	1.27476000	-0.45543900
H	2.53614000	-2.60846100	0.50686000
H	2.28413000	2.14398200	-0.78844300
H	4.46443100	1.14826400	-0.23314700
H	-4.47143000	1.48302700	-0.11933700
H	-2.22975500	2.31859900	-0.69907800
N	-0.02245400	0.95126000	-0.83696400
H	0.02733100	2.00603600	-0.74787600
O	0.08353300	3.32835800	0.02775700
O	0.94256300	3.18165100	1.07884100
H	0.36700100	3.06980000	1.84528800
S	-0.13104700	-2.07926400	-0.17547500
N	4.87847300	-1.36262800	0.53378100
H	4.94591700	-2.36370100	0.47135200
H	5.69615900	-0.89126400	0.18753500
N	-5.07063900	-1.00410600	0.60238600
H	-5.85200200	-0.47216900	0.25932200
H	-5.21221200	-1.99616600	0.51955900
Name of species		PC: 3,7-di-NH ₂ -PhtzN.....H-OOH	
0 2			
C	-3.86839100	-0.61030500	0.01770800
C	-2.77751800	-1.47526400	0.04398400
C	-1.47854500	-0.98194100	0.02250900
C	-1.22013400	0.40752800	-0.02373300
C	-2.34940200	1.26112800	-0.04987400
C	-3.63148700	0.77639400	-0.02700300
C	1.14892100	0.26911100	-0.02716400
C	1.23931200	-1.14155500	0.00900300
C	2.46990300	-1.78618900	0.01393700
H	2.50633700	-2.86840700	0.04438500
C	3.65513100	-1.05558700	-0.01432400
C	3.58431000	0.35034900	-0.03751900
C	2.37001100	0.98611900	-0.04621700
H	-2.94190600	-2.54514600	0.08469700
H	-2.16462200	2.32632700	-0.08714900
H	-4.47049800	1.45966200	-0.04080000
H	4.49858200	0.92939100	-0.04467300
H	2.30952400	2.06636100	-0.05373200
N	0.00269400	0.99346200	-0.04782900
H	0.06414800	2.76122300	-0.31116600
O	0.06846100	3.74452500	-0.42116100
O	1.19150600	4.11238400	0.37537500

H	0.77248500	4.48920400	1.15411100
S	-0.18484500	-2.15976000	0.05016700
N	-5.16231100	-1.09610800	0.08496400
H	-5.88653600	-0.48283100	-0.24563000
H	-5.29806500	-2.05632900	-0.17844500
N	4.88256700	-1.69152000	0.03309900
H	4.90295200	-2.65671800	-0.24576400
H	5.67207400	-1.16141500	-0.29170900
3,7-di-CF ₃ -PhtzNH + HOO•			
Name of species		RC: 3,7-di-CF ₃ -PhtzN-H..... OOH	
0 2			
C	-3.69036100	-0.34436600	0.10750800
C	-2.61987700	-1.11604300	-0.32992000
C	-1.40662900	-0.51164500	-0.61390600
C	-1.24026800	0.86251200	-0.41114100
C	-2.31684000	1.62164300	0.04467000
C	-3.54229000	1.02388800	0.28960400
C	1.18524200	0.79341900	-0.41099700
C	1.27228400	-0.58822000	-0.61421600
C	2.44932100	-1.26145800	-0.33278200
H	2.50251400	-2.33183500	-0.47750400
C	3.56300500	-0.55308700	0.10417000
C	3.49312000	0.82109600	0.28781200
C	2.30377800	1.48916800	0.04459400
H	-2.73626000	-2.18142100	-0.47397500
H	-2.18699600	2.68454800	0.20051900
H	-4.37814800	1.61901500	0.62717500
H	4.36211500	1.36664700	0.62531200
H	2.23834100	2.55803900	0.19904300
N	-0.00934200	1.46496600	-0.66668300
H	0.01737300	2.45537600	-0.47240300
O	0.00236000	4.54730800	0.01849200
O	1.22181000	4.99842900	0.12104400
H	1.14836500	5.94996900	0.30445800
S	-0.09267100	-1.44473800	-1.35111700
C	4.81560100	-1.29427100	0.43897700
C	-4.98344600	-1.01119100	0.44533000
F	-4.99450500	-1.47953900	1.71073900
F	-5.23156200	-2.06504400	-0.35261400
F	-6.02771400	-0.17111400	0.33862000
F	5.02010200	-2.33757200	-0.38506500
F	4.78531800	-1.79706400	1.69073900
F	5.90298700	-0.50676200	0.36841700
Name of species		TS: 3,7-di-CF ₃ -PhtzN...H...OOH	
0 2			
C	-3.79669000	-0.28204700	-0.02460400
C	-2.69313400	-1.10576000	0.07588600
C	-1.41373900	-0.57715200	-0.08645900
C	-1.24781900	0.78729200	-0.35985500
C	-2.38745800	1.60462000	-0.45955500
C	-3.64751700	1.08083500	-0.29017100
C	1.18464700	0.75096100	-0.38528800

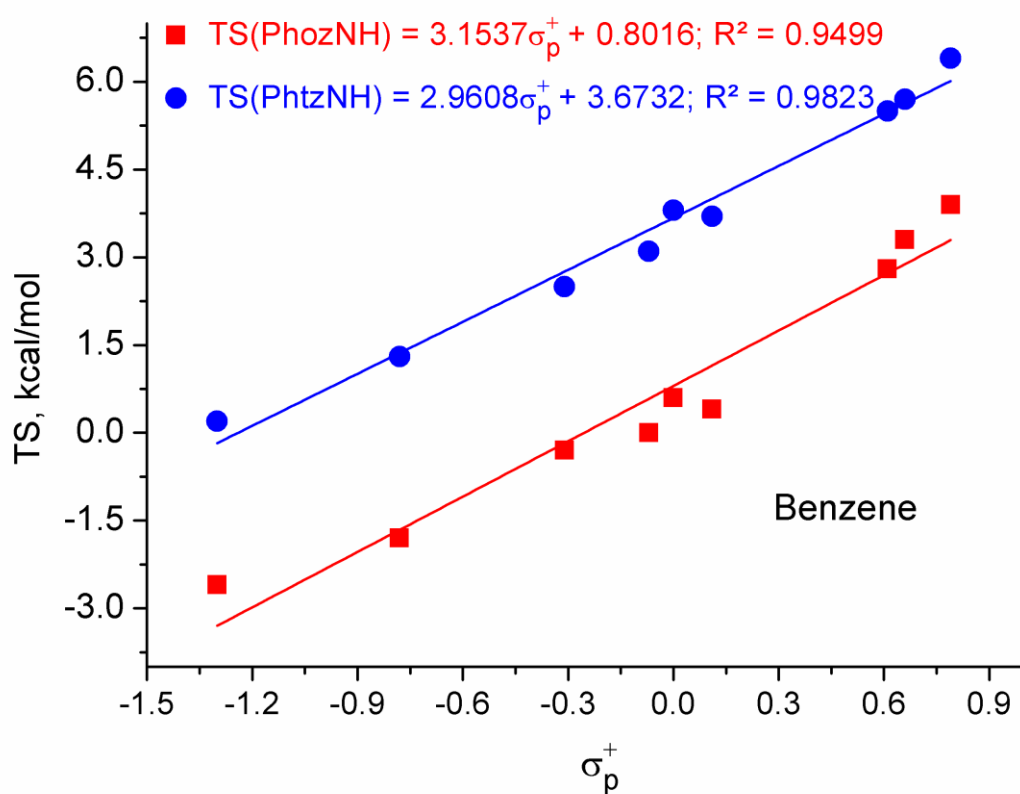
C	1.30846100	-0.61970100	-0.09862900
C	2.56963100	-1.18981500	0.04729100
H	2.66114700	-2.24423700	0.26849100
C	3.70199500	-0.40917400	-0.09578700
C	3.59755600	0.95000200	-0.38968600
C	2.35297900	1.51958700	-0.53816500
H	-2.81784500	-2.15820000	0.28937800
H	-2.24649100	2.65730500	-0.66227100
H	-4.51828300	1.71733000	-0.36031600
H	4.48925500	1.54794800	-0.51172400
H	2.24928700	2.56913200	-0.76914600
N	-0.02189600	1.38835100	-0.55207800
H	-0.02864500	2.48105200	-0.31728800
O	-0.16979100	3.64721600	0.38584100
O	1.09099000	4.10867100	0.67148500
H	1.07935000	4.23151700	1.62791300
S	-0.06903100	-1.69768700	0.03564300
C	-5.17908000	-0.83437900	0.12645700
C	5.06065200	-1.00270500	0.10737000
F	-5.17711600	-2.10899700	0.54456600
F	-5.85531500	-0.79833400	-1.03732200
F	-5.89964700	-0.12086300	1.00999400
F	5.92936700	-0.57786000	-0.82599400
F	5.57780000	-0.65463300	1.30136400
F	5.04240800	-2.34373400	0.06270100
Name of species		PC: 3,7-di-CF ₃ -PhtzN.....H-OOH	
O 2			
C	-3.78909600	-0.33877000	-0.00378300
C	-2.69693100	-1.17643200	0.00504700
C	-1.40931600	-0.63391400	-0.00983300
C	-1.21319600	0.76768400	-0.03153200
C	-2.36920200	1.59204400	-0.04175700
C	-3.62857600	1.05603600	-0.02777000
C	1.15488100	0.72081000	-0.03166600
C	1.29158300	-0.68789000	-0.01550500
C	2.55503200	-1.28400800	-0.00723400
H	2.64604700	-2.36140900	0.00369700
C	3.68002200	-0.49088200	-0.01358600
C	3.57696800	0.90941200	-0.02568100
C	2.34155200	1.49973700	-0.03468100
H	-2.83234500	-2.24897500	0.02150000
H	-2.21686400	2.66234400	-0.06005100
H	-4.49900300	1.69732300	-0.03700000
H	4.47312100	1.51434900	-0.02762600
H	2.23038200	2.57563300	-0.03107800
N	-0.01680200	1.39749000	-0.04489900
H	-0.02470300	3.22503200	-0.29098100
O	-0.05041200	4.20079900	-0.39508600
O	1.11414300	4.58546300	0.33054300
H	0.73745400	5.04178800	1.08845900
S	-0.08142000	-1.75610300	-0.00668900
C	-5.17919500	-0.89334600	0.02617800

C	5.04673100	-1.10115900	0.00809900
F	-5.82683500	-0.52945200	1.14817600
F	-5.19696200	-2.23307900	-0.02861100
F	-5.91101700	-0.43719400	-1.00523500
F	5.01017800	-2.44098100	-0.03999900
F	5.71756800	-0.75845200	1.12304100
F	5.78805200	-0.68049600	-1.03148800
3,7-di-CN-PhtzNH + HOO [•]			
Name of species		RC: 3,7-di-CN-PhtzN–H..... OOH	
0 2			
C	3.73698000	-0.58585200	-0.30454200
C	2.67551000	-1.42831400	0.03047300
C	1.44591000	-0.88968100	0.36606400
C	1.24718800	0.49497300	0.32022400
C	2.30885800	1.32875900	-0.03289300
C	3.55078800	0.79611900	-0.32721700
C	-1.18065600	0.37069300	0.32356800
C	-1.23653600	-1.02700200	0.37015700
C	-2.40538200	-1.68897800	0.03803300
H	-2.43736700	-2.76936400	0.05436000
C	-3.54876400	-0.96022400	-0.29431400
C	-3.50454700	0.43346400	-0.31844900
C	-2.32289600	1.09101900	-0.02834600
H	2.81907700	-2.49955200	0.04631700
H	2.15135500	2.39857900	-0.06986000
H	4.37480200	1.44355000	-0.58901500
H	-4.39138500	0.99289000	-0.57809600
H	-2.27855600	2.17144800	-0.06682100
N	0.00260400	1.03796100	0.62532000
H	-0.04719300	2.04313000	0.54079300
O	-0.02071700	4.14293100	0.12347000
O	-1.20717200	4.60774300	-0.15203700
H	-1.09412000	5.55340600	-0.34646300
S	0.15625700	-1.93842500	0.97820000
C	5.01588600	-1.14366500	-0.62447500
C	-4.76498100	-1.64549500	-0.61101400
N	6.04294900	-1.58877000	-0.88158400
N	-5.74237800	-2.19199000	-0.86623700
Name of species		TS: 3,7-di-CN-PhtzN...H...OOH	
0 2			
C	-3.82881800	-0.50257000	0.00866800
C	-2.72864900	-1.34309700	0.12682500
C	-1.44367600	-0.83761300	-0.02983600
C	-1.25443500	0.52472100	-0.31271700
C	-2.37993000	1.35829400	-0.42950200
C	-3.65100600	0.85882800	-0.26777800
C	1.17544300	0.45037700	-0.32854100
C	1.27825300	-0.92281000	-0.03403100
C	2.52716800	-1.50957600	0.11673300
H	2.60608700	-2.56305800	0.34788200
C	3.68075700	-0.74568900	-0.02546900
C	3.59190000	0.61745700	-0.32777000

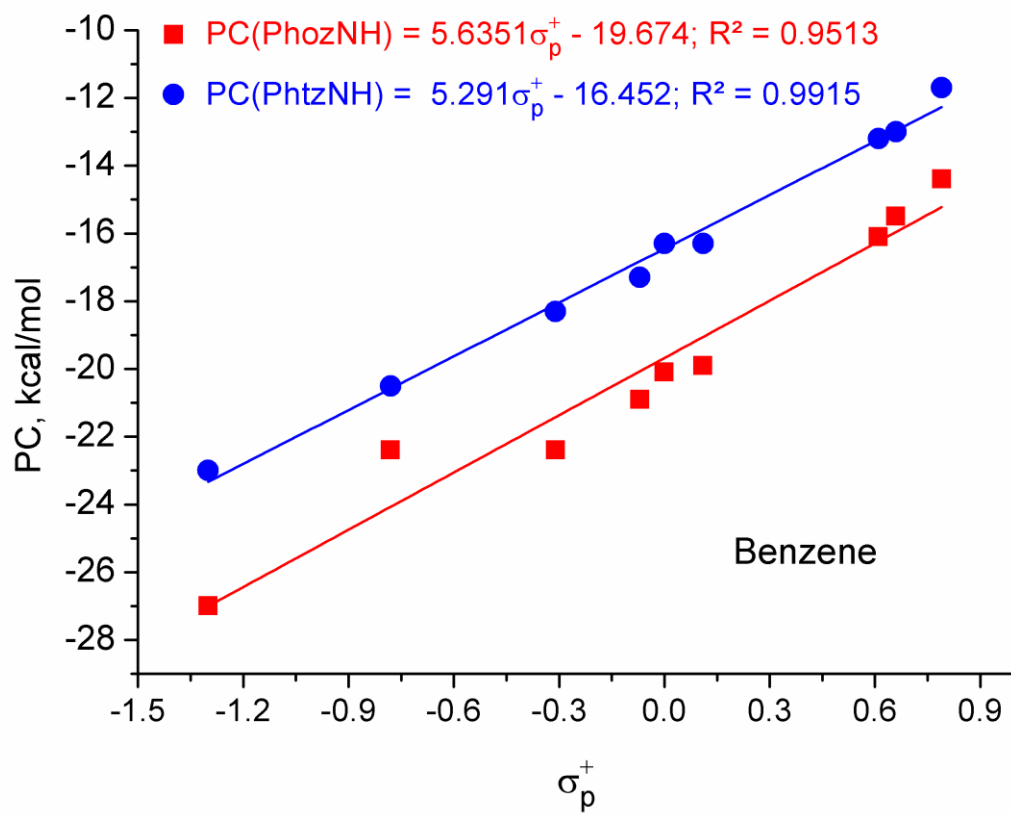
C	2.35526500	1.20121300	-0.48207500
H	-2.87501500	-2.39190500	0.34606600
H	-2.22096500	2.40664100	-0.64146800
H	-4.51108900	1.50589900	-0.35491700
H	4.49286200	1.20111400	-0.44412400
H	2.26763700	2.25181600	-0.71537300
N	-0.01935000	1.10365200	-0.49834800
H	-0.01147000	2.20849300	-0.28682500
O	-0.14246700	3.39103600	0.36408000
O	1.12102400	3.85625000	0.63164400
H	1.09987100	4.04616300	1.57692200
S	-0.11668800	-1.97772400	0.10702900
C	-5.14734000	-1.03583800	0.17380200
C	4.96239200	-1.36311300	0.13731700
N	-6.20517500	-1.46251400	0.30593000
N	5.99119400	-1.85590600	0.26953700
Name of species		PC: 3,7-di-CN-PhtzN.....H-OOH	
O 2			
C	-3.82872400	-0.54762600	0.01476600
C	-2.74599400	-1.41298600	0.02177700
C	-1.45002700	-0.90327000	0.00559100
C	-1.22093300	0.49630500	-0.01607700
C	-2.35598400	1.34793700	-0.02418400
C	-3.62931700	0.84613000	-0.00976500
C	1.14479800	0.39745500	-0.01853800
C	1.25114500	-1.01669400	-0.00420500
C	2.49767700	-1.63661400	0.00096400
H	2.57023600	-2.71574700	0.01062800
C	3.65021900	-0.86661500	-0.00613800
C	3.57144500	0.53917100	-0.01541400
C	2.34650300	1.15140200	-0.02102200
H	-2.91090200	-2.48173600	0.03910500
H	-2.17784300	2.41424900	-0.04175200
H	-4.48420800	1.50614500	-0.01672700
H	4.47983900	1.12346500	-0.01679200
H	2.25786500	2.22948700	-0.01425600
N	-0.01161500	1.09679000	-0.02973800
H	0.02254900	2.92906100	-0.29769700
O	0.02814800	3.90223600	-0.41726000
O	1.18984100	4.26125300	0.32615700
H	0.81434400	4.76392900	1.05480300
S	-0.14642300	-2.05474800	0.00546900
C	-5.15734700	-1.07874400	0.03253900
C	4.92786200	-1.51122700	-0.00011400
N	-6.22473500	-1.50172200	0.04744000
N	5.95335400	-2.02772000	0.00557500
3,7-di-NO ₂ -PhtzNH + HOO [•]			
Name of species		RC: 3,7-di-NO ₂ -PhtzN-H..... OOH	
O 2			
C	3.69973600	-0.45946500	-0.20377800
C	2.64462000	-1.29717300	0.12733700
C	1.42111600	-0.73499800	0.44432600

C	1.24569500	0.65347700	0.37787200
C	2.32269900	1.46963300	0.02595100
C	3.56016400	0.91805400	-0.25134800
C	-1.18576800	0.56918100	0.37954800
C	-1.26409700	-0.82810000	0.44668100
C	-2.44615600	-1.47435400	0.13242400
H	-2.51881000	-2.55147900	0.15955000
C	-3.55787800	-0.71264000	-0.19677200
C	-3.51406700	0.67117600	-0.24600000
C	-2.31735200	1.30814700	0.02771200
H	2.79328400	-2.36639700	0.15387500
H	2.17993000	2.54072800	-0.02523000
H	4.40603200	1.53327600	-0.51590100
H	-4.40122000	1.22586400	-0.50901900
H	-2.25215900	2.38668400	-0.02522000
N	0.00895900	1.22103900	0.65928300
H	-0.02441700	2.22631000	0.56509800
O	0.01945100	4.30702700	0.12425700
O	-1.16837400	4.76820700	-0.15077800
H	-1.05666800	5.71092400	-0.36034900
S	0.11328500	-1.75732000	1.06134700
N	5.00126800	-1.05518000	-0.51403800
N	-4.81558000	-1.39740000	-0.50390000
O	5.90534700	-0.30418400	-0.80711000
O	5.09307700	-2.26123500	-0.45950800
O	-5.76989900	-0.71112000	-0.79588400
O	-4.82376700	-2.60689600	-0.44816400
Name of species		TS: 3,7-di-NO ₂ -PhtzN...H...OOH	
O 2			
C	-3.78850100	-0.37957100	-0.03829200
C	-2.70410100	-1.22349200	0.08930500
C	-1.42372100	-0.69930100	-0.04492800
C	-1.24831700	0.66961400	-0.31207300
C	-2.38149700	1.49334900	-0.43590400
C	-3.65029800	0.98025800	-0.29561500
C	1.18037300	0.62036900	-0.32452900
C	1.29615900	-0.75691000	-0.04746800
C	2.55099600	-1.33700500	0.08232400
H	2.66334300	-2.38947500	0.29884700
C	3.67333500	-0.54568900	-0.06550000
C	3.59693800	0.81306600	-0.34589300
C	2.35189100	1.38537800	-0.48032000
H	-2.86315700	-2.27201400	0.29599800
H	-2.23061900	2.54483800	-0.63708400
H	-4.52743500	1.60178500	-0.38441500
H	4.50114600	1.38977200	-0.46012300
H	2.25126400	2.43751000	-0.70027400
N	-0.01981200	1.26561800	-0.47606800
H	-0.02630200	2.37612800	-0.23295900
O	-0.16927100	3.52332200	0.43311600
O	1.09231400	4.00064900	0.69114900
H	1.07756700	4.18555700	1.63758900

S	-0.08662700	-1.82258300	0.10913400
N	-5.13680400	-0.94469500	0.10888700
N	4.99496700	-1.17202100	0.07898600
O	-6.07170600	-0.18683200	-0.01043500
O	-5.22370700	-2.12952100	0.33885400
O	5.96347500	-0.45823800	-0.04448700
O	5.02792600	-2.35881700	0.31267900
Name of species			PC: 3,7-di-NO ₂ -PhtzN.....H-OOH
O 2			
C	3.64626100	-0.64312000	-0.00455800
C	2.52807600	-1.44462800	-0.00162100
C	1.27352700	-0.83883800	-0.00595900
C	1.14994100	0.57520400	-0.01532700
C	2.34114600	1.34715800	-0.01428700
C	3.57597300	0.75324800	-0.00906200
C	-1.21590700	0.64264400	-0.01484800
C	-1.42440900	-0.76161000	0.00109900
C	-2.71324000	-1.29140800	0.01412900
H	-2.88662400	-2.35798100	0.02703000
C	-3.78273600	-0.42585600	0.00945400
C	-3.63006600	0.96398500	-0.00937800
C	-2.36203600	1.48100200	-0.02046800
H	2.63736600	-2.51961700	0.00419700
H	2.23680700	2.42363900	-0.00431600
H	4.48550400	1.33332500	-0.00723500
H	-4.50483500	1.59552200	-0.01381700
H	-2.19711700	2.54932800	-0.03373900
N	-0.01526500	1.25850700	-0.02548500
H	-0.00443300	3.09885000	-0.29820100
O	-0.00745000	4.07047200	-0.42205700
O	1.15034100	4.44206300	0.32144300
H	0.77071500	4.95746100	1.03898000
S	-0.10759900	-1.89471400	-0.00151300
N	4.96684000	-1.29014400	0.00101300
N	-5.13868700	-0.99272300	0.02447700
O	5.93613000	-0.56814600	0.00237300
O	4.99595800	-2.50001900	0.00414800
O	-5.23981500	-2.19841600	0.03574200
O	-6.06331400	-0.21361200	0.02537800



a)



b)

Figure S1. Correlation between the modified Hammett parameters with **(a)** TS energy barriers, and **(b)** PC reaction energies in the reaction of $\text{HOO}^\bullet$ with PhozNHs and PhtzNHs in benzene (at M05-2X-GD3/6-311+G(d,p) + ZPE).

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