THEORETICAL EVALUATION OF HEXAZINANE AS A BASIC COMPONENT OF NITROGEN-RICH ENERGETIC ONIUM SALTS

Sergey V. Bondarchuk

Department of Chemistry and Nanomaterials Science,

Bogdan Khmelnitsky Cherkasy National University,

blvd. Shevchenko 81, 18031 Cherkasy, Ukraine.

Tel: (+3) 80472 37-65-76;

Fax: (+3) 80472 37-21-42;

E-mail: bondchem@cdu.edu.ua

Molecular Systems Design & Engineering

SUPPORTING INFORMATION

LIST OF SUPPLEMENTARY FIGURES, TABLES AND EQUATIONS:

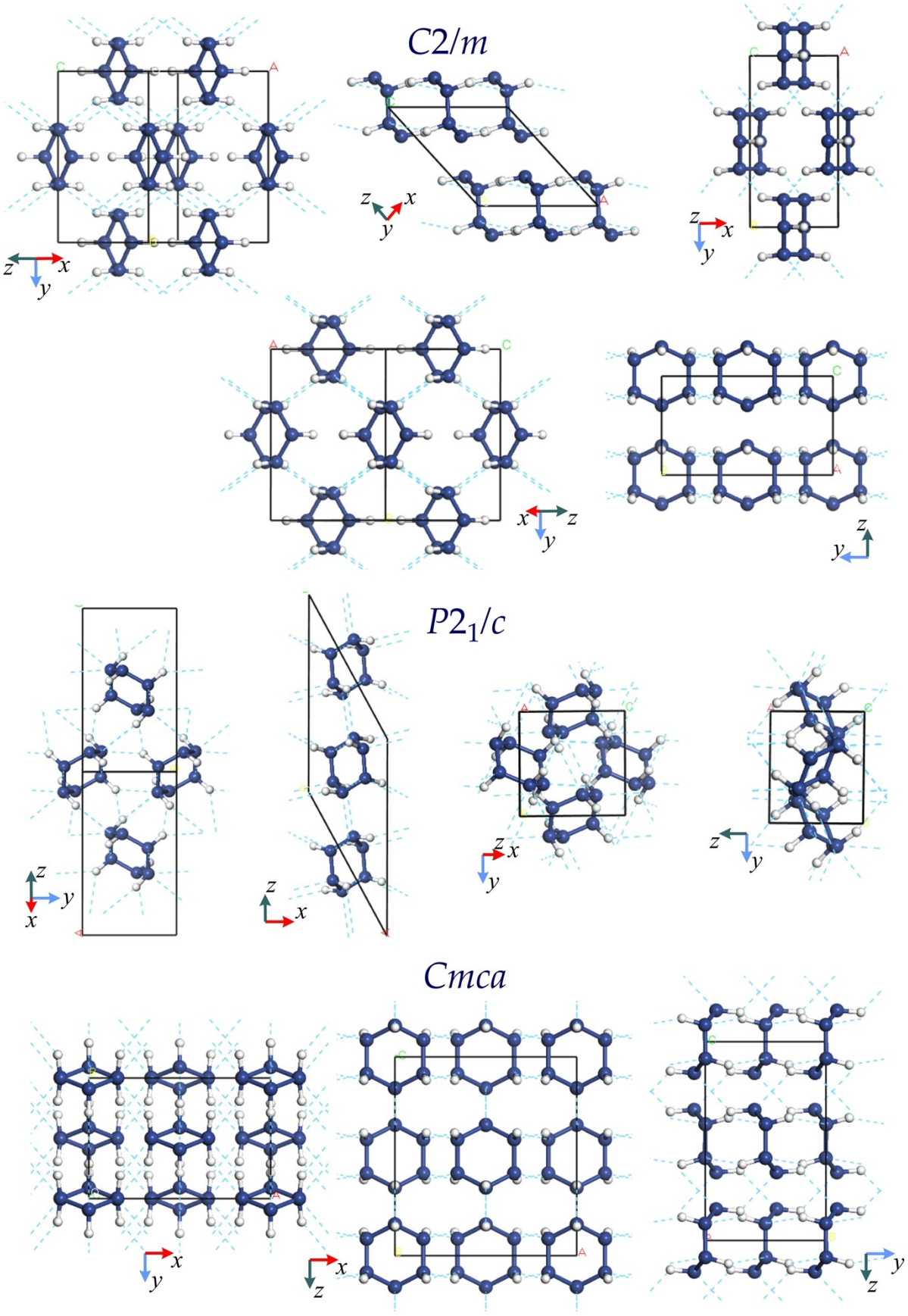


Figure S1. Different projections of a unit cell of three *a,a,a,a,a,a* polymorphs of hexazinane.

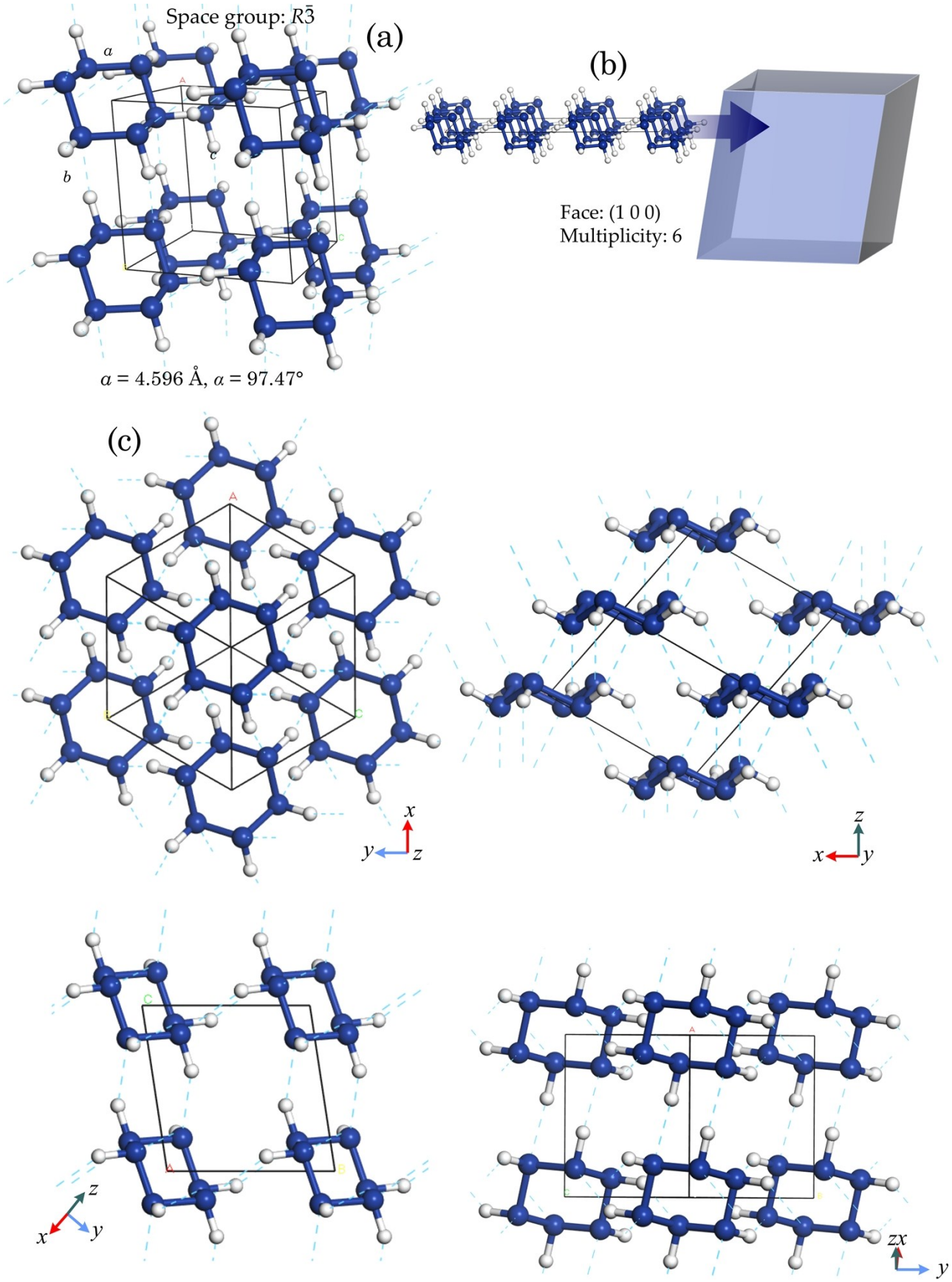


Figure S2. Different projections of the *e*,*e*,*e*,*e*,*e*,*e* polymorph of hexazinane.

Table S1. Fractional coordinates of atoms for hexazinane polymorphs

Space group	Atom	*x*	*y*	*z*	Wyckoff position
*C*2/*m*	N1	0.612	0	0.294	4i
	N2	0.616	0.159	0.165	8j
	H3	0.389	0	0.254	4i
	H4	0.861	0.173	0.245	8j
$P2_1/c$	N1	0.310	0.194	0.278	4e
	N2	0.280	0.201	0.405	4e
	N3	0.572	0.077	0.691	4e
	H4	0.484	0.352	0.374	4e
	H5	0.068	0.072	0.274	4e
	H6	0.782	0.217	0.839	4e
Cmca	N1	0	0.591	-0.342	8f
	N2	0.156	0.493	-0.415	16g
	H3	0	0.788	-0.352	8f
	H4	0.171	0.308	-0.383	16g
$R\bar{3}$	N1	0.826	0.115	0.199	18f
	H2	0.605	0.089	0.235	18f

Table S2. The selected crystal habit parameters in vacuum predicted by the attachment energy method

Space group	*hkl*	Multiplicity	d_{hkl} (Å)	% Area	% Total area	Vertices
*C*2/*m*	(1 -1 1)	4	0.996	17.208	68.833	4
	(1 1 -1)	2	1.100	15.584	31.167	4
$P2_1/c$	(2 0 -2)	2	0.260	34.273	68.546	4
	(0 1 1)	4	1.131	7.864	31.454	4
Cmca	(1 -1 2)	4	1.638	18.864	75.455	4
	(1 1 0)	2	2.518	12.272	24.545	4

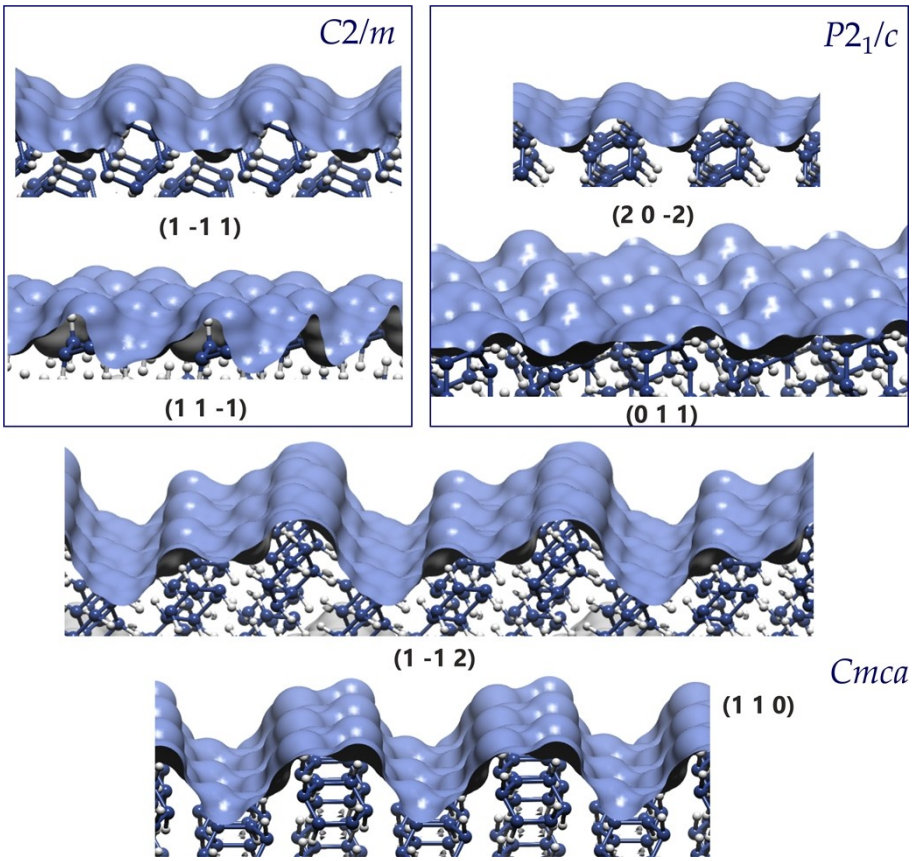
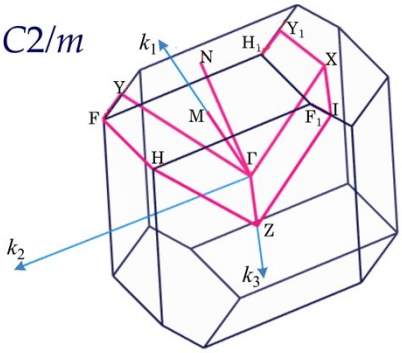


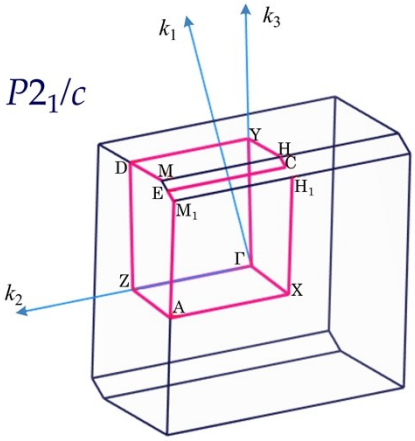
Figure S3. Stable surfaces of crystal habits of the predicted hexazinane polymorphs

Monoclinic

*C*2/*m*



*P*2$_1$/*c*



The Born-Huang criteria for the Laue class 2, *m*, 2/*m*

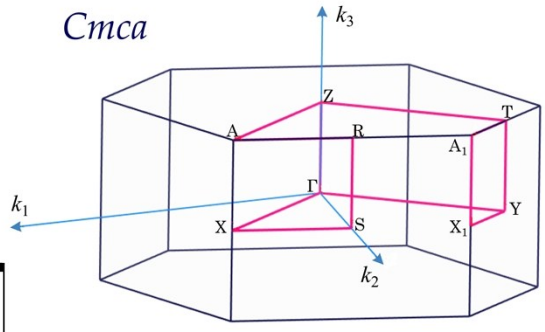
$$\begin{cases} C_{11}>0 \\ C_{44}>0 \\ C_{11}C_{22}-C_{12}^2>0 \\ C_{44}C_{66}-C_{46}^2>0 \\ T=C_{11}C_{22}C_{33}+2C_{12}C_{13}C_{23}-C_{11}C_{23}^2-C_{22}C_{13}^2-C_{33}C_{12}^2>0 \\ C_{15}^2(C_{23}^2-C_{22}C_{33})+C_{25}^2(C_{13}^2-C_{11}C_{33})+C_{35}^2(C_{12}^2-C_{11}C_{22}) \\ +2C_{15}C_{35}(C_{13}C_{22}-C_{12}C_{23})+2C_{15}C_{25}(C_{12}C_{33}-C_{13}C_{23}) \\ +2C_{25}C_{35}(C_{23}C_{11}-C_{12}C_{13})+C_{55}T>0 \end{cases}$$

Equation for the 3D Young's modulus plotting

$$\frac{1}{E}=l_1^4s_{11}+2l_1^2l_2^2s_{12}+2l_1^2l_3^2s_{13}+2l_1^3l_3s_{15}+l_2^4s_{22}+2l_2^2l_3^2s_{23}+2l_1l_2^2l_3s_{25}$$
$$+l_3^4s_{33}+2l_1l_3^3s_{35}+l_2^2l_3^2s_{44}+2l_1l_2^2l_3s_{46}+l_1^2l_3^2s_{55}+l_1^2l_2^2s_{66}$$

Orthorhombic

Cmca



The Born-Huang criteria for the Laue class *mmm*

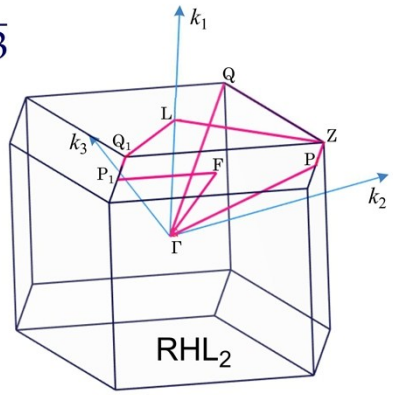
$$\begin{cases} C_{11}>0;\ C_{11}C_{22}>C_{12}^2 \\ C_{11}C_{22}C_{33}+2C_{12}C_{13}C_{23}-C_{11}C_{23}^2-C_{22}C_{13}^2-C_{33}C_{12}^2>0 \\ C_{44}>0;\ C_{55}>0;\ C_{66}>0 \end{cases}$$

Equation for the 3D Young's modulus plotting

$$\frac{1}{E}=l_1^4s_{11}+2l_1^2l_2^2s_{12}+2l_1^2l_3^2s_{13}+l_2^4s_{22}+2l_2^2l_3^2s_{23}+l_3^4s_{33}+l_2^2l_3^2s_{44}+l_1^2l_3^2s_{55}+l_1^2l_2^2s_{66}$$

Trigonal

$R\bar{3}$



The Born-Huang criteria for the Laue class $\bar{3}$

$$\begin{cases} C_{11}>|C_{12}|;\ C_{44}>0; \\ C_{13}^2<1/2C_{33}(C_{11}+C_{12}); \\ C_{14}^2+C_{15}^2<1/2C_{44}(C_{11}-C_{12})\equiv C_{44}C_{66}. \end{cases}$$

Equation for the 3D Young's modulus plotting

$$\frac{1}{E}=(1-l_3^2)^2s_{11}+l_3^4s_{33}+l_3^2(1-l_3^2)(2s_{13}+s_{44})+$$
$$+2l_2l_3(3l_1^2-l_2^2)s_{14}+(2l_1l_3(3l_2^2-l_1^2)s_{25}$$

where $l_1=\sin\theta\cos\varphi \quad l_2=\sin\theta\sin\varphi \quad l_3=\cos\theta$

Figure S4. Dynamical and mechanical stability criteria for different Laue classes.

Table S3. The calculated elastic stiffness constants C_{ij} (GPa) of hexazinane polymorphs

C*2/*m	C_{ij}	1	2	3	4	5	6
	1	42.06260	4.01355	5.89313		8.91792	
	2	4.01355	64.15315	16.56287		-19.13245	
	3	5.89313	16.56287	44.31510		-3.46890	
	4				36.23525		-6.22105
	5	8.91792	-19.13245	-3.46890		42.73995	
	6				-6.22105		20.21690
	S_{ij}	1	2	3	4	5	6
	1	0.0259387	-0.0029551	-0.0028905		-0.0069697	
	2	-0.0029551	0.0201496	-0.0064245		0.0091151	
	3	-0.0028905	-0.0064245	0.0253343		-0.0002166	
	4				0.0291367		0.0089658
	5	-0.0069697	0.0091151	-0.0002166		0.0289144	
	6				0.0089658		0.0522225
P*2$_1$/*c	C_{ij}	1	2	3	4	5	6
	1	40.99780	1.60782	22.01420		1.59407	
	2	1.60782	40.85040	11.79897		-3.35288	
	3	22.01420	11.79897	43.39145		4.03962	
	4				23.70325		-5.32393
	5	1.59407	-3.35288	4.03962		9.37185	
	6				-5.32393		15.18345
	S_{ij}	1	2	3	4	5	6
	1	0.0342371	0.0044474	-0.0189454		0.0039339	
	2	0.0044474	0.0287949	-0.0114337		0.0144736	
	3	-0.0189454	-0.0114337	0.0373463		-0.0169657	
	4				0.0457949		0.0160575
	5	0.0039339	0.0144736	-0.0169657		0.1185243	
	6				0.0160575		0.0714916
Cmca	C_{ij}	1	2	3	4	5	6
	1	121.48335	55.85190	33.48770			
	2	55.85190	51.44285	30.38327			
	3	33.48770	30.38327	45.45550			
	4				14.08230		
	5					19.42625	
	6						4.74650
	S_{ij}	1	2	3	4	5	6
	1	0.0164378	-0.0176701	-0.0002990			
	2	-0.0176701	0.0511138	-0.0211476			
	3	-0.0002990	-0.0211476	0.0363552			
	4				0.0710111		
	5					0.0514767	
	6						0.2106816
***R*$\bar{3}$**	C_{ij}	1	2	3	4	5	6
	1	53.93	-13.63	11.29	7.91	-5.75	
	2						
	3			46.22			
	4				18.89		
	5						
	6						
	S_{ij}	1	2	3	4	5	6
	1	0.0230781	0.0056656	-0.0070189	-0.0072903	0.0053047	
	2						
	3			0.0250654			
	4				0.0622836		
	5						
	6						

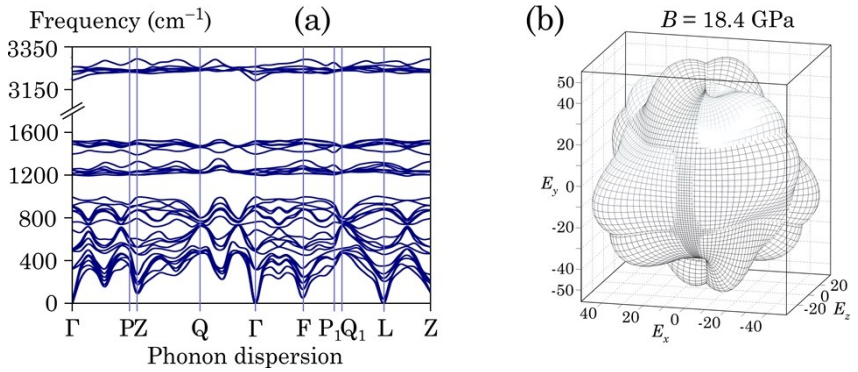


Figure S5. Phonon dispersion and 3D presentation of the Young modulus for the *e,e,e,e,e,e* polymorph of hexazinane.

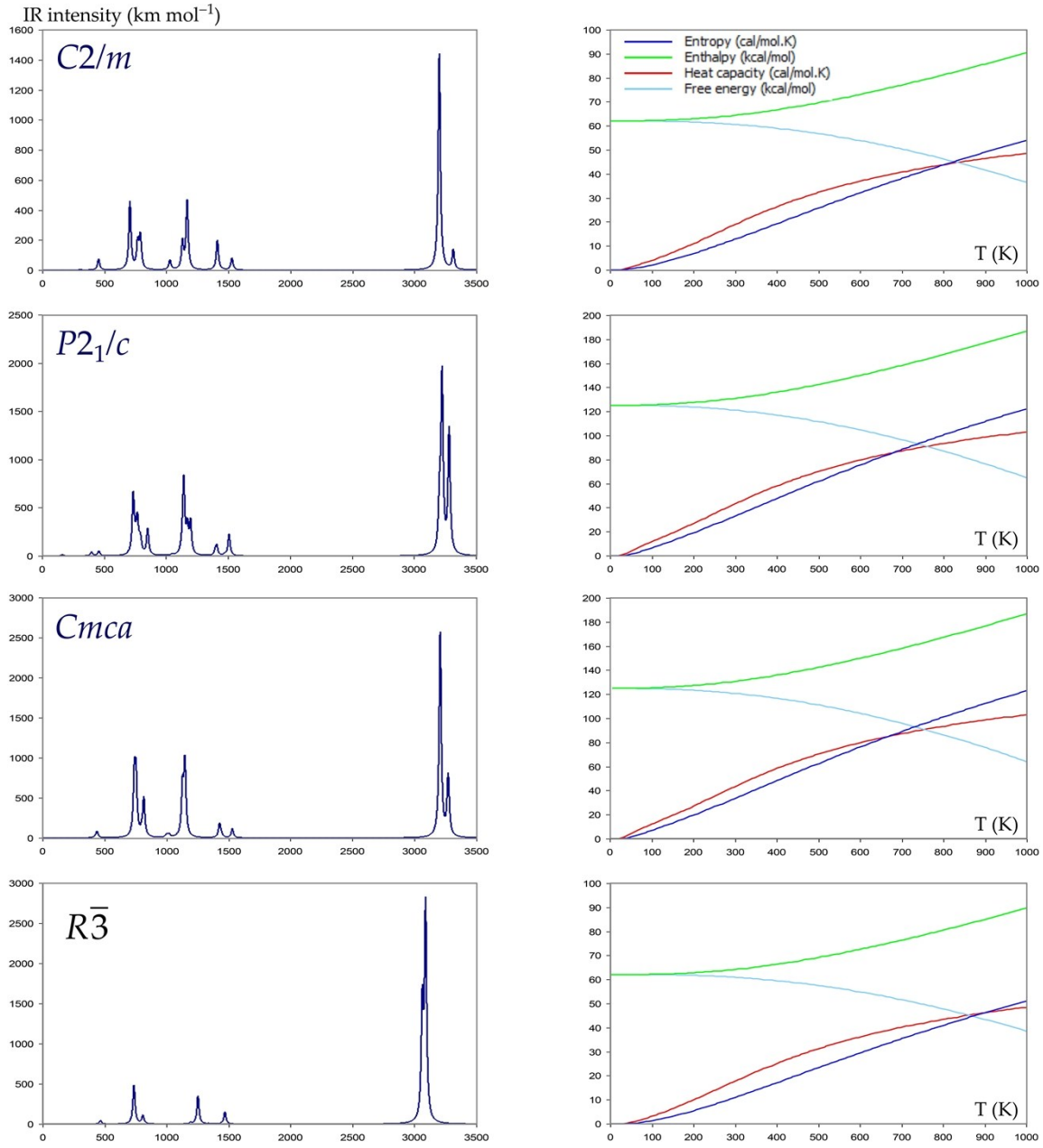


Figure S6. The calculated IR spectra along with the temperature dependence of main thermodynamic functions of hexazinane polymorphs.

Table S4. Comparison of the prediction of the gas phase enthalpies of formation for the benchmark set molecules

Molecule	ΔH_{gas}, kJ mol^{-1} (calculated)	ΔH_{gas}, kJ mol^{-1} (experimental)	Δ, kJ mol^{-1}
NH_3	-46.4	-45.9[a]	0.5
NH_2NH_2	94.6	95.4[a]	0.8
NH_2OH	-41.2	-50.2[b]	9.0
CH_3NH_2	-23.4	-23.5[a]	-0.1
$(CH_3)_2NH$	-16.4	-19.0[a]	-2.6
HNO_3	-136.4	-134.3[a]	2.1
HNO_2	-77.7	-76.7[a]	1.0
NO_2	15.6	33.1[a]	17.5
NO	82.5	90.3[a]	7.8
H_2O	-233.0	-241.8[a]	-8.8
CH_3NO_2	-80.3	-81.0[a]	-0.7
CH_3CH_2OH	-228.4	-234.0[a]	-5.6
CH_3COOH	-430.0	-433.0[a]	-3.0
HCl	-91.5	-92.3[a]	-0.8
CH_3Cl	-83.8	-81.9[a]	1.9
NOCl	40.2	51.7[a]	11.5
RDX	208.0	192.0[a]	-16.0
TNT	23.5	24.1[a]	0.6
Nitroglycerin	-276.7	-279.1[a]	-2.4
1*H*-Tetrazole	320.3	320.0[a]	-0.3

[a]The values are taken from the NIST Chemistry WebBook (https://webbook.nist.gov/chemistry/)
[b]The value is taken from L. V. Gurvich et al. *Thermodynamic Properties of Individual Substances*, 4th ed., Hemisphere Publishing Corp., 1989, Vol. 1 and 2.

Table S5. Comparison of the prediction of the solid state enthalpies of formation for the benchmark set crystals

Crystal	ΔH_{gas}, kJ mol^{-1}	ΔH_{sub}, kJ mol^{-1}	ΔH_{solid}, kJ mol^{-1} (calculated)	ΔH_{solid}, kJ mol^{-1} (experimental)	Δ, kJ mol^{-1}
NH_4Cl	-165.7	142.8	-308.5	-314.6	-6.1
NH_4NO_3	-229.7	169.3	-399.0	-365.1	33.9
TKX-50	479.8	363.9	115.9	114.0	1.9

Table S6. The relative energies (kJ mol^{-1}) of salts 1-10 in several space groups predicted by Polymorph

Salt	*C*2/*c*	*P*-1	$P2_1/c$	$P2_1$	$P2_12_12_1$	*Pbca*	$Pna2_1$
1	11.1	14.3	7.1	13.5	5.6	0.0	6.8
2	4.2	6.0	1.3	0.9	2.7	4.5	0.0
3	9.1	3.2	1.2	2.6	3.3	0.4	0.0
4	12.0	12.3	0.8	0.0	1.6	0.2	0.1
5	18.9	15.8	10.2	8.4	1.0	2.9	0.0
6	44.8	24.8	38.3	17.5	0.0	8.8	11.4
7	17.0	17.5	2.3	4.1	0.0	6.7	4.8
8	25.2	19.7	10.0	10.4	2.6	0.0	2.6
9	11.9	7.8	0.0	7.4	6.7	6.9	6.1
10	20.4	14.2	11.8	5.3	1.4	8.0	0.0

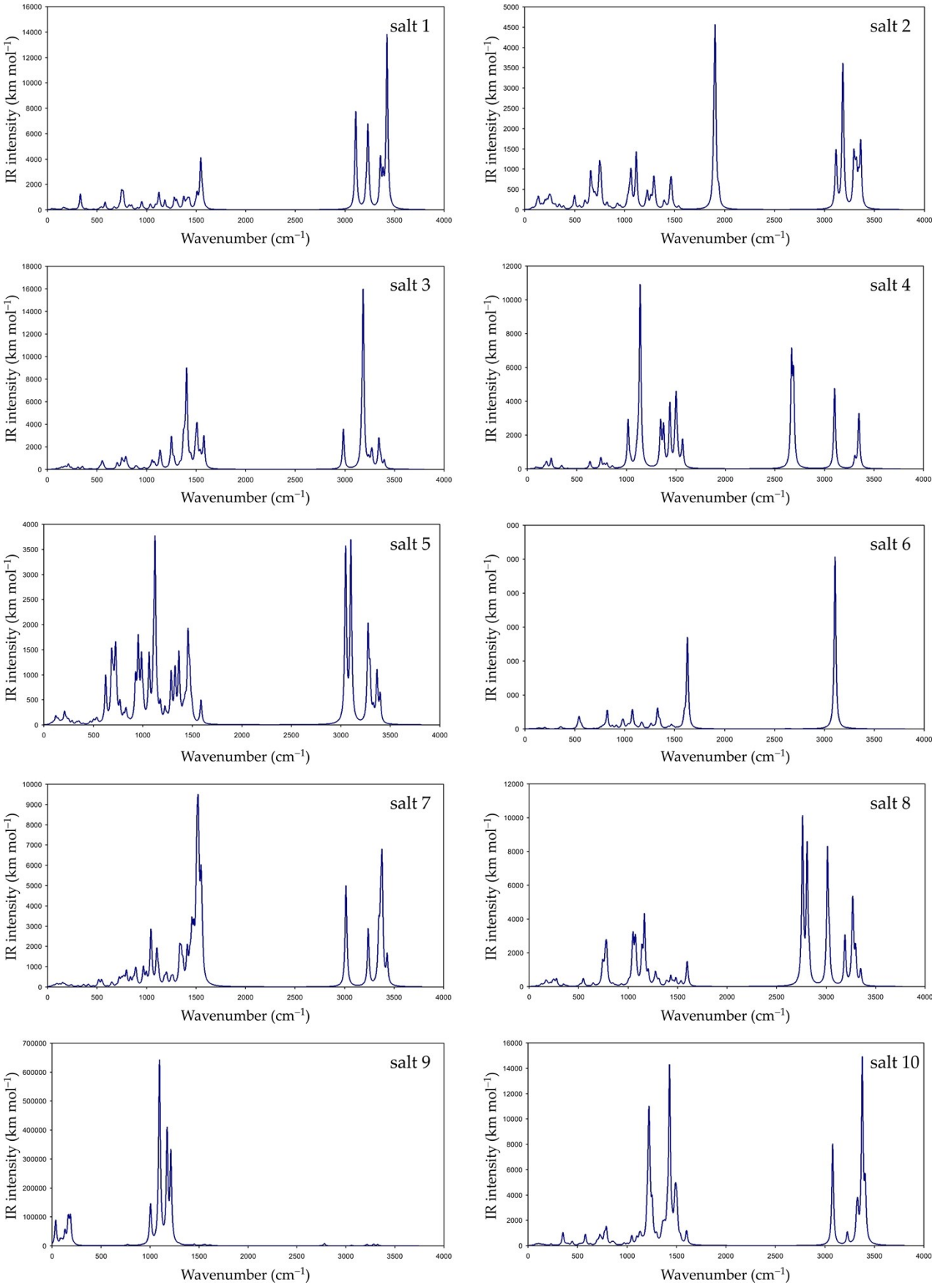


Figure S7. The calculated IR spectra of salts **1**-**10**.

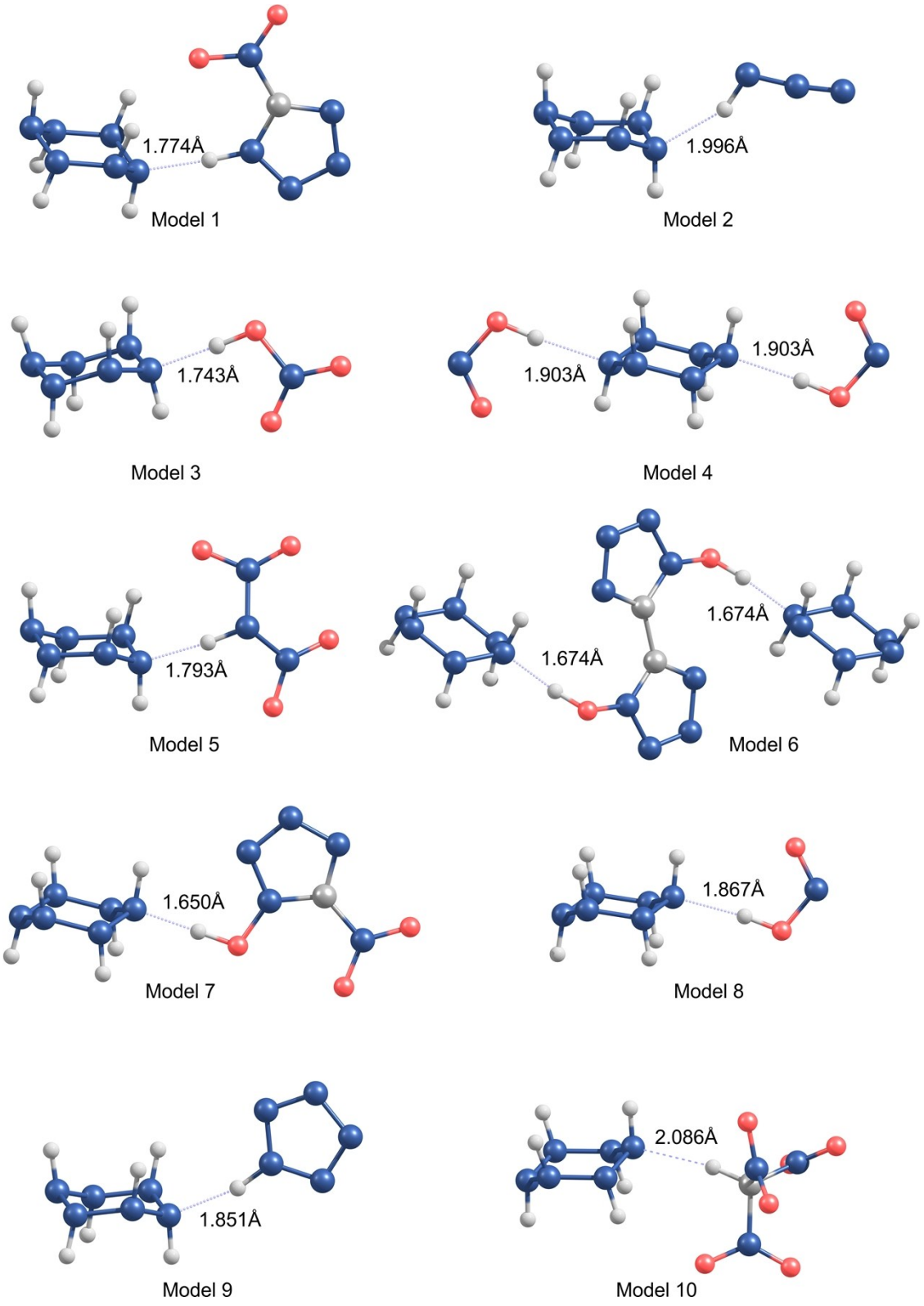


Figure S8. Finite size models used for the gas phase enthalpy of formation and lattice energy calculations.

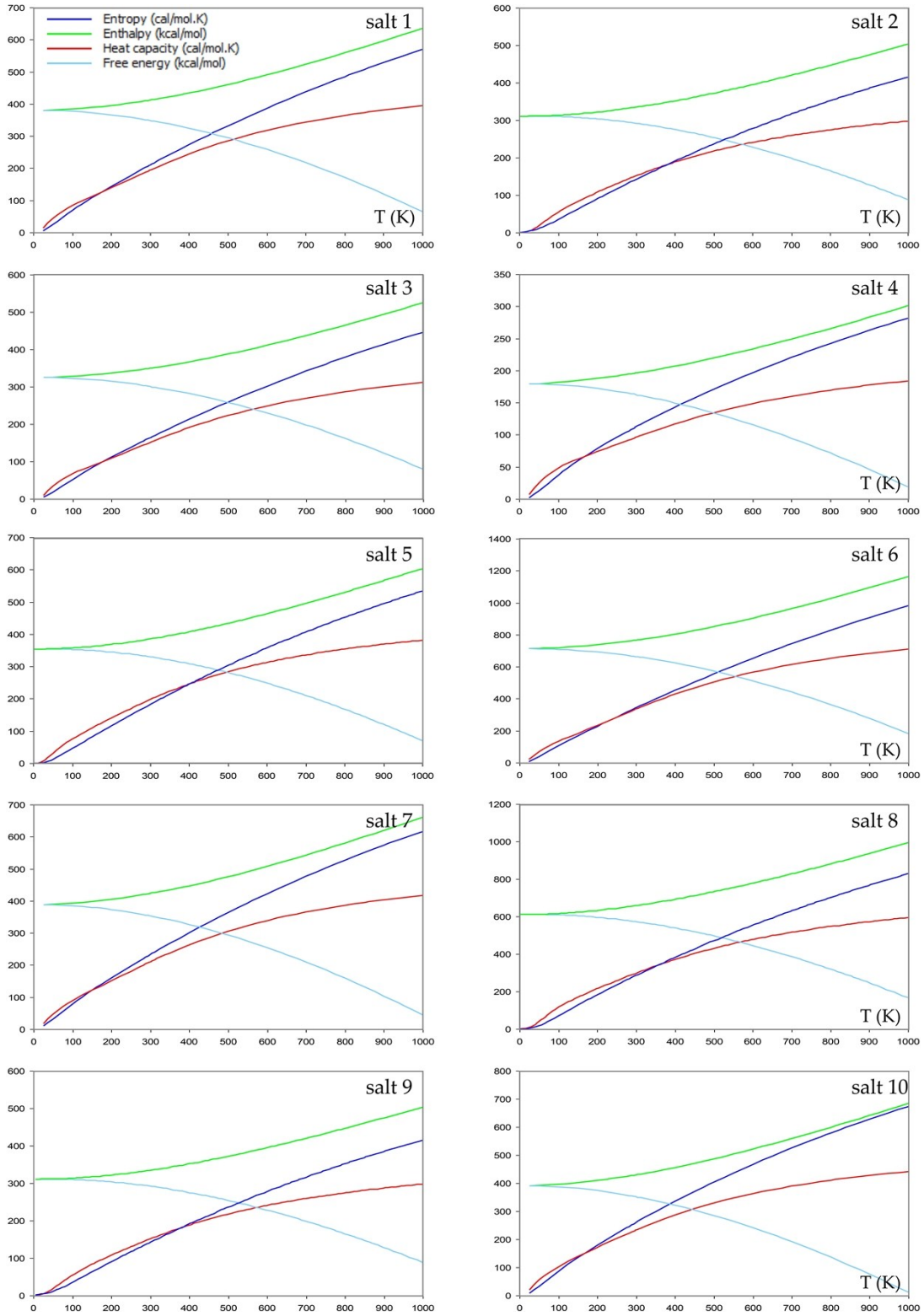


Figure S9. Temperature dependence of the main thermodynamic functions of salts **1**-**10**.

Coefficients of the NASA polynomials for hexazinane and its salts in the formatted form for the CEA2 program

```
H6N6              Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 1 Dec/19 H   6.00N   6.00    0.00    0.00    0.00 1   90.0878400     439700.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         12196.042
-3.552439260D+05 6.156136460D+03-4.356000070D+01 1.817575380D-01-2.259181146D-04
 1.455140326D-07-3.772561810D-11 0.000000000D+00 2.325185666D+04 2.297899787D+02
```

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Salt1             Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 1 Dec/19 C   1.00H   7.00N  11.00O   2.00    0.00 1  205.1387800     750300.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6637.941
 1.272835103D+07-1.198458147D+05 2.566974936D+02 4.605933430D-01-1.998386217D-03
 2.333236107D-06-8.997446070D-10 0.000000000D+00 7.322272550D+05-1.849192256D+03

Salt2             Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 1 Dec/19 H   7.00N   9.00    0.00    0.00    0.00 1  133.1158800     701100.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        24265.161
-3.478719230D+05 5.254732410D+03-3.190361690D+01 1.750455437D-01-2.043713653D-04
 1.241267951D-07-3.036493107D-11 0.000000000D+00 5.652283600D+04 1.711431500D+02

Salt3             Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 1 Dec/19 H   7.00N   7.00O   3.00    0.00    0.00 1  153.1006800     221300.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5247.734
 9.643813680D+06-9.129089510D+04 1.967377107D+02 3.513887180D-01-1.528484431D-03
 1.787600568D-06-6.899554940D-10 0.000000000D+00 5.151220290D+05-1.415567202D+03

Salt4             Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 1 Dec/19 H   8.00N   8.00O   4.00    0.00    0.00 1  184.1147200     263100.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7468.396
 1.295779434D+07-1.287451828D+05 3.262359320D+02 2.595143934D-01-1.733127253D-03
 2.158744470D-06-8.534975530D-10 0.000000000D+00 7.112893590D+05-2.223332121D+03

Salt5             Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 1 Dec/19 H   7.00N   9.00O   4.00    0.00    0.00 1  197.1134800     481000.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        31258.339
 1.543992483D+05-1.223050608D+03-1.226854843D+00 1.269707098D-01-1.295600055D-04
 6.508213320D-08-1.226394799D-11 0.000000000D+00 6.108114550D+04-6.319962360D+00

Salt6             Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 1 Dec/19 C   2.00H  14.00N  20.00O   2.00    0.00 1  350.2653600    1419300.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10497.699
 2.229405358D+07-2.072253383D+05 4.258471760D+02 8.672448860D-01-3.565888370D-03
 4.122229580D-06-1.583256357D-09 0.000000000D+00 1.284755542D+06-3.112030222D+03

Salt7             Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 1 Dec/19 C   1.00H   7.00N  11.00O   3.00    0.00 1  221.1381800     683900.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7227.936
 1.405172449D+07-1.315530799D+05 2.757588401D+02 5.375173600D-01-2.260542907D-03
 2.617564506D-06-1.004842452D-09 0.000000000D+00 7.880848060D+05-2.001675062D+03

Salt8             Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 2 Dec/19 H   7.00N   7.00O   2.00    0.00    0.00 0  137.1012800     355800.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        24451.084
-4.470808490D+05 6.889352600D+03-4.067491480D+01 1.944414684D-01-2.264705444D-04
 1.371925074D-07-3.356825950D-11 0.000000000D+00 7.270884570D+03 2.212444294D+02

Salt9             Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 1 Dec/19 H   7.00N  11.00    0.00    0.00    0.00 1  161.1292800     773500.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5401.678
 1.001997316D+07-9.719097040D+04 2.354615622D+02 2.215677250D-01-1.304179189D-03
 1.607478988D-06-6.352160790D-10 0.000000000D+00 6.089869480D+05-1.623093802D+03

Salt10            Sergey V. Bondarchuk, Dec/19, Mol. Syst. Des. Eng.
 1 Dec/19 C   1.00H   7.00N   9.00O   6.00    0.00 1  241.1229800     398500.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8251.008
 1.583795415D+07-1.484310569D+05 3.096260899D+02 6.261106040D-01-2.610747721D-03
 3.010672740D-06-1.152227270D-09 0.000000000D+00 8.442657740D+05-2.253888564D+03
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Table S7. Decomposition schemes corresponding to the maximum propulsive performance

Crystal	O/F	Decomposition equation
H_6N_6	0	$H_6N_6 = 3\ N_2 + 3\ H_2$
	0.2667	$8\ H_6N_6 + 6\ O_2 = 48\ N_2 + 12\ H_2O + 12\ H_2$
Salt1	0	$2\ CH_7N_{11}O_2 = CO + CO_2 + H_2O + 6\ H_2 + 11\ N_2$
	0.0975	$8\ CH_7N_{11}O_2 + 5\ O_2 = 4\ CO + 4\ CO_2 + 14\ H_2O + 14\ H_2 + 44\ N_2$
Salt2	0	$2\ H_7N_9 = 9\ N_2 + 7\ H_2$
	0.2103	$8\ H_7N_9 + 7\ O_2 = 36\ N_2 + 14\ H_2O + 14\ H_2$
Salt3	0	$2\ H_7N_7O_3 = 7\ N_2 + 6\ H_2O + H_2$
Salt4	0	$H_8N_8O_4 = 4\ N_2 + 4\ H_2O$
Salt5	0	$4\ H_7N_9O_4 = 18\ N_2 + 14\ H_2O + O_2$
Salt6	0	$5C_2H_{14}N_{20}O_2 = 50\ N_2 + 33\ H_2 + 2\ H_2O + 4\ CO + 4\ C + 2\ CO_2$
	0.2284	$2\ C_2H_{14}N_{20}O_2 + 5\ O_2 = 2\ CO + 2\ CO_2 + 8\ H_2O + 6\ H_2 + 20\ N_2$
Salt7	0	$2\ CH_7N_{11}O_3 = CO + CO_2 + 3\ H_2O + 4\ H_2 + 11\ N_2$
	0.0724	$2\ CH_7N_{11}O_2 + O_2 = CO + CO_2 + 5\ H_2O + 2\ H_2 + 11\ N_2$
Salt8	0	$2\ H_7N_7O_2 = 7\ N_2 + 4\ H_2O + 3\ H_2$
	0.0525	$40\ H_7N_7O_2 + 9\ O_2 = 140\ N_2 + 98\ H_2O + 42\ H_2$
Salt9	0	$2\ H_7N_{11} = 11\ N_2 + 7\ H_2$
	0.1986	$2\ H_7N_{11} + 2\ O_2 = 11\ N_2 + 4\ H_2O + 3\ H_2$
Salt10	0	$4\ CH_7N_9O_6 = 4\ CO_2 + 14\ H_2O + 18\ N_2 + O_2$

Table S8. Mole fractions of species formed upon decomposition of the studied salts at various Ae/At ratios of FAC

O/F	Species	Injector	Combustion chamber end Ae/At = 1.58	Throat Ae/At = 1	Exit Ae/At = 10	Exit Ae/At = 25	Exit Ae/At = 50	Exit Ae/At = 68.9
				H_6N_6				
0	H•	0.01338	0.01177	0.00482				
	H_2	0.48996	0.49117	0.49638	0.49999	0.49992	0.49887	0.49591
	N_2	0.49665	0.49706	0.49879	0.50000	0.50000	0.50000	0.50000
0.2667	H•	0.07919	0.07752	0.06518	0.00037			
	H_2	0.22019	0.22032	0.22316	0.24949	0.24971	0.24972	0.24972
	H_2O	0.19658	0.19867	0.21023	0.25022	0.25028	0.25028	0.25028
	N_2	0.46753	0.46854	0.47469	0.49990	0.50000	0.50000	0.50000
	OH•	0.02588	0.02491	0.01981	0.00002			
				Salt1				
0	CO	0.09178	0.09185	0.09246	0.08396	0.06859	0.05042	0.04109
	CO_2	0.00465	0.00473	0.00510	0.01604	0.03141	0.04958	0.05882
	H•	0.06021	0.05781	0.04252				
	H_2	0.22193	0.22312	0.23120	0.26603	0.28141	0.29956	0.30855
	H_2O	0.08166	0.08250	0.08671	0.08396	0.06859	0.05043	0.04131
	N_2	0.52982	0.53078	0.53633	0.55000	0.55000	0.55001	0.55012
0.0975	CO	0.08136	0.08126	0.08105	0.07340	0.06241	0.04944	0.04211
	CO_2	0.01178	0.01207	0.01345	0.02655	0.03759	0.05056	0.05789
	H•	0.07311	0.07170	0.06119	0.00083	0.00001		
	H_2	0.13076	0.13056	0.13069	0.15111	0.16258	0.17555	0.18288
	H_2O	0.14336	0.14536	0.15700	0.19828	0.18742	0.17445	0.16712
	N_2	0.50931	0.51048	0.51759	0.54975	0.55000	0.55000	0.55000
	OH•	0.03065	0.02975	0.02494	0.00007			

Table S8. ***Continue***

O/F	Species	Injector	Combustion chamber end Ae/At = 1.58	Throat Ae/At = 1	Exit Ae/At = 10	Exit Ae/At = 25	Exit Ae/At = 50	Exit Ae/At = 68.9
				Salt2				
0	H•	0.03490	0.03225	0.01835				
	H_2	0.41241	0.41432	0.42431	0.43750	0.43749	0.43743	0.43726
	N_2	0.55268	0.55343	0.55734	0.56250	0.56250	0.56250	0.56251
0.2103	H•	0.08840	0.08669	0.07410	0.00092	0.00001		
	H_2	0.19002	0.19006	0.19227	0.21825	0.21878	0.21879	0.21879
	H_2O	0.15840	0.16049	0.17218	0.21854	0.21871	0.21871	0.21871
	N_2	0.52063	0.52182	0.52904	0.56222	0.56250	0.56250	0.56250
	OH•	0.02820	0.02729	0.02250	0.00006			
				Salt3				
0	H•	0.03625	0.03543	0.02923	0.00029			
	H_2	0.10293	0.10187	0.09605	0.07133	0.07143	0.07143	0.07143
	H_2O	0.33036	0.33322	0.35043	0.42838	0.42857	0.42857	0.42857
	N_2	0.46722	0.46822	0.47414	0.49990	0.50000	0.50000	0.50000
	OH•	0.03863	0.03748	0.03135	0.00010			
				Salt4				
0	H•	0.03365	0.03289	0.02718	0.00086	0.00003		
	H_2	0.07646	0.07532	0.06840	0.01060	0.00168	0.00018	0.00005
	H_2O	0.34019	0.34313	0.36123	0.48351	0.49762	0.49975	0.49993
	NO•	0.01067	0.01024	0.00864	0.00069	0.00009	0.00001	
	N_2	0.45344	0.45447	0.46051	0.49614	0.49947	0.49995	0.49999
	O•	0.01262	0.01227	0.00987	0.00021	0.00001		
	OH•	0.05061	0.04940	0.04323	0.00389	0.00040	0.00003	0.00001
	O_2	0.02233	0.02226	0.02092	0.00409	0.00070	0.00008	0.00002
				Salt5				
0	H•	0.04126	0.04041	0.03386	0.00137	0.00004		
	H_2	0.06510	0.06411	0.05808	0.00702	0.00057	0.00002	
	H_2O	0.26939	0.27215	0.28914	0.40863	0.42245	0.42408	0.42420
	NO•	0.01576	0.01519	0.01328	0.00256	0.00082	0.00022	0.00010
	N_2	0.48849	0.48969	0.49671	0.54008	0.54461	0.54531	0.54539
	O•	0.02205	0.02155	0.01816	0.00119	0.00009		
	OH•	0.06186	0.06064	0.05468	0.00946	0.00173	0.00021	0.00006
	O_2	0.03606	0.03623	0.03607	0.02969	0.02969	0.03015	0.03024
				Salt6				
0	CO	0.10350	0.10364	0.10434	0.10440	0.07944	0.05004	0.03745
	CO_2	0.00001	0.00001	0.00001	0.00024	0.00953	0.02090	0.02550
	H•	0.03021	0.02775	0.01515				
	H_2	0.34755	0.34925	0.35791	0.36768	0.36004	0.35261	0.34876
	H_2O	0.00018	0.00016	0.00013	0.00043	0.00699	0.01376	0.01722
	N_2	0.51837	0.51902	0.52233	0.52657	0.52747	0.52803	0.52834
	$C_{(gr)}$				0.00043	0.01542	0.03303	0.04080
0.2284	CO	0.08303	0.08289	0.08248	0.07466	0.06520	0.05376	0.04719
	CO_2	0.01382	0.01415	0.01582	0.03044	0.04006	0.05150	0.05807
	H•	0.07634	0.07507	0.06527	0.00267	0.00009		
	H_2	0.12437	0.12402	0.12309	0.13445	0.14526	0.15675	0.16332
	H_2O	0.15761	0.15975	0.17245	0.23184	0.22310	0.21167	0.20510
	N_2	0.48052	0.48168	0.48868	0.52548	0.52629	0.52632	0.52632
	O•	0.01287	0.01241	0.00952	0.00001			
	OH•	0.03761	0.03667	0.03176	0.00043			

Table S8. ***Continue***

O/F	Species	Injector	Combustion chamber end Ae/At = 1.58	Throat Ae/At = 1	Exit Ae/At = 10	Exit Ae/At = 25	Exit Ae/At = 50	Exit Ae/At = 68.9
				Salt7				
0	CO	0.08377	0.08370	0.08368	0.07387	0.06000	0.04424	0.03580
	CO_2	0.01092	0.01116	0.01228	0.02612	0.04000	0.05576	0.06420
	H•	0.06407	0.06253	0.05138	0.00012			
	H_2	0.14617	0.14621	0.14792	0.17606	0.19000	0.20576	0.21420
	H_2O	0.14183	0.14362	0.15372	0.17386	0.16000	0.14424	0.13580
	N_2	0.51875	0.51986	0.52648	0.54996	0.55000	0.55000	0.55000
	OH•	0.02272	0.02183	0.01709				
0.0724	CO	0.07449	0.07424	0.07317	0.05997	0.05134	0.04145	0.03596
	CO_2	0.01733	0.01776	0.02001	0.03983	0.04865	0.05855	0.06404
	H•	0.06225	0.06118	0.05290	0.00291	0.00012		
	H_2	0.09763	0.09708	0.09444	0.08877	0.09852	0.10848	0.11397
	H_2O	0.17175	0.17396	0.18734	0.25866	0.25139	0.24151	0.23603
	N_2	0.50038	0.50159	0.50884	0.54889	0.54996	0.55000	0.55000
	O•	0.01487	0.01439	0.01134	0.00002			
	OH•	0.04173	0.04075	0.03576	0.00087	0.00001		
	O_2	0.01029	0.01017	0.00894	0.00002			
				Salt8				
0	H•	0.05174	0.05030	0.03998	0.00003			
	H_2	0.19887	0.19883	0.20030	0.21427	0.21429	0.21429	0.21429
	H_2O	0.24342	0.24550	0.25685	0.28571	0.28571	0.28571	0.28571
	N_2	0.47734	0.47826	0.48371	0.49999	0.50000	0.50000	0.50000
	OH•	0.02116	0.02017	0.01485				
0.0525	H•	0.05554	0.05443	0.04586	0.00039			
	H_2	0.15309	0.15245	0.14997	0.14982	0.15001	0.15002	0.15002
	H_2O	0.27188	0.27449	0.28972	0.34985	0.34998	0.34998	0.34998
	N_2	0.46733	0.46834	0.47444	0.49989	0.50000	0.50000	0.50000
	OH•	0.03462	0.03351	0.02755	0.00005			
				Salt9				
0	H•	0.03028	0.02781	0.01515				
	H_2	0.36786	0.36957	0.37836	0.38889	0.38888	0.38881	0.38860
	N_2	0.60186	0.60261	0.60648	0.61111	0.61111	0.61112	0.61114
0.1986	H•	0.07706	0.07551	0.06419	0.00070	0.00001		
	H_2	0.15266	0.15241	0.15256	0.16627	0.16665	0.16666	0.16666
	H_2O	0.15619	0.15839	0.17089	0.22209	0.22223	0.22223	0.22223
	N_2	0.56660	0.56789	0.57571	0.61088	0.61111	0.61111	0.61111
	OH•	0.02997	0.02906	0.02422	0.00006			
				Salt10				
0	CO	0.05753	0.05691	0.05339	0.01456	0.00382	0.00047	0.00011
	CO_2	0.03908	0.03987	0.04456	0.09139	0.10368	0.10754	0.10796
	H•	0.03426	0.03366	0.02867	0.00318	0.00054	0.00004	0.00001
	H_2	0.04815	0.04752	0.04344	0.01112	0.00333	0.00052	0.00015
	H_2O	0.24192	0.24407	0.25761	0.35112	0.36998	0.37674	0.37778
	NO•	0.01696	0.01635	0.01432	0.00330	0.00151	0.00063	0.00037
	N_2	0.42625	0.42735	0.43361	0.47512	0.48300	0.48572	0.48615
	O•	0.02476	0.02424	0.02065	0.00251	0.00058	0.00008	0.00002
	OH•	0.06184	0.06063	0.05487	0.01399	0.00535	0.00148	0.00065
	O_2	0.04921	0.04935	0.04885	0.03371	0.02820	0.02678	0.02679