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Supporting Information

Theoretical performance evaluation of hypergolic ionic liquid fuels with storable oxidizers

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ESI-1: The sample output of NASA-CEC 71 of IL [AEIM][BH_3CN] with WFNA.

```
 INPUT FILE NAME FLI(PROP DATA):il125w.d

 INPUT FILE NAME FLS(CONTROL)  :bhi2.d

 OUTPUT FILE NAME FLO          :il125w.o

REACTANTS

   C    9.00H   16.00N    3.00B    1.00     .00   100.00  56660.10   298.15     .95LF

   N    1.00H    1.00O    3.00      .00     .00   100.00 -41610.00   298.15    1.48LO

NAME

SPECIES BEING CONSIDERED IN THIS SYSTEM

   J12/64  B(S)        J12/64  B(L)        J12/64  B           J12/64  BH          J12/64  BH2

   J12/64  BH3         J 6/66  BN(S)       J 6/66  BN          J 6/68  BO          J 6/68  BO2

   J12/64  B2          J 6/66  B2O         J24/91  BO2H        J20/91  BO2H2       J27/91  BO3H3(S)

   J25/91  BO3H3       J14/91  B2O4H4      J12/91  B2H6        J 5/91  B3N3H6      J12/64  B2O2

   J12/64  B2O3(L)     J12/64  B2O3        J17/91  B3O3H3(S)   J 6/91  B3O3H3      J18/91  B3H3O6

   J 7/91  B4C(S)      J13/91  B5H9        J20/91  B10H14(L)   J 8/91  B10H14      J 3/61  C(S)

   J 3/61  C           J12/67  CH          J 6/69  CH2         J 3/61  CH2O        J 6/69  CH3

   J 3/61  CH4         J 6/69  CN          J 6/66  CN2         J 9/65  CO          J 9/65  CO2

   J12/69  C2          J 3/67  C2H         J 3/61  C2H2        J 9/65  C2H4        J 3/67  C2N

   J 3/61  C2N2        J 9/66  C2O         J12/69  C3          J 6/68  C3O2        J12/69  C4

   J12/69  C5          J 9/65  H           J12/64  HBO         J12/64  HBO2        000000  HCN

   J 3/61  HCO         J 3/63  HNO         J 3/64  HO2         J 3/61  H2          L11/65  H2O(S)

   L11/65  H2O(L)      J 3/61  H2O         L 2/69  H2O2        J12/64  H3B3O6      J 3/61  N

   J12/65  NH          J12/65  NH2         J 9/65  NH3         J 6/63  NO          J 9/64  NO2

   J 9/65  N2          J 6/66  N2C         J12/65  N2H4        J12/64  N2O         J 9/64  N2O4

   J 6/62  O           J 3/66  OH          J 9/65  O2


OF =   2.500000

                  EFFECTIVE FUEL     EFFECTIVE OXIDANT       MIXTURE

ENTHALPY              HPP(2)              HPP(1)             HSUB0

(KG-MOL)(DEG K)/KG     .16103690E+03      -.33230770E+03      -.19135210E+03

KG-ATOMS/KG            B0P(I,2)            B0P(I,1)             B0(I)

     C              .50830510E-01       .00000000E+00       .14523000E-01
```

H	.90365350E-01	.15869990E-01	.37154380E-01
N	.16943500E-01	.15869990E-01	.16176710E-01
B	.56478340E-02	.00000000E+00	.16136670E-02
O	.00000000E+00	.47609980E-01	.34007130E-01

PT C H N B O

1 -14.388 -9.871 -13.417 -17.560 -17.321 5.000

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 2.53830 MPA

CASE NO. 1

		WT FRACTION	ENERGY	STATE	TEMP	DENSITY
	CHEMICAL FORMULA	(SEE NOTE)	CAL/MOL		DEG K	G/CC
FUEL	C 9.00000 H 16.00000 N 3.00000 B 1.00000	1.00000	56660.100	L	298.15	.9533
OXIDANT	N 1.00000 H 1.00000 O 3.00000	1.00000	-41610.000	L	298.15	1.4800

O/F= 2.5000 PERCENT FUEL= 28.5714 EQUIVALENCE RATIO= 1.4716 REACTANT DENSITY= 1.2782

	CHAMBER	THROAT	EXIT	EXIT
PC/P	.1000E+01	.1786E+01	.2500E+02	.2460E+02
P MPA	.2538E+01	.1421E+01	.1015E+00	.1032E+00
T DEG K	.3018E+04	.2716E+04	.1647E+04	.1653E+04
RHO G/CC	.2375E-02	.1477E-02	.1740E-03	.1763E-03
H CAL/G	-.3803E+03	-.5206E+03	-.9987E+03	-.9964E+03
S CAL/G/K	.2676E+01	.2676E+01	.2676E+01	.2676E+01
M MOL WT	.2351E+02	.2351E+02	.2351E+02	.2351E+02
CP CAL/G K	.4676E+00	.4622E+00	.4276E+00	.4279E+00
GAMMA (S)	.1221E+01	.1224E+01	.1246E+01	.1246E+01
SON VEL M/S	.1141E+04	.1084E+04	.8519E+03	.8532E+03
MACH NO.	.0000E+00	.1000E+01	.2670E+01	.2661E+01
AE/AT		.1000E+01	.4045E+01	.4000E+01
C* M/S		.1583E+04	.1583E+04	.1583E+04
CF		.6851E+00	.1438E+01	.1435E+01

IVAC KG-S/KG .2008E+03 .2581E+03 .2578E+03

ISP KG-S/KG .1105E+03 .2320E+03 .2315E+03

MOLE FRACTIONS

BO	.2883E-03	BO2	.6907E-03	BO2H	.1835E-01	BO3H3	.3467E-04
B2O3	.3047E-03	CO	.2574E+00	CO2	.8400E-01	H	.1153E-01
HBO	.5630E-05	HBO2	.1796E-01	HCO	.4675E-04	H2	.1214E+00
H2O	.2867E+00	NO	.1233E-02	N2	.1896E+00	O	.5418E-03
OH	.9288E-02	O2	.5176E-03				

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .50000E-05 FOR ALL ASSINGED CONDITIONS

B(S) B(L) B BH BH2 BH3 BN(S) BN B2 B2O

BO2H2 BO3H3(S) B2O4H4 B2H6 B3N3H6 B2O2 B2O3(L) B3O3H3(S) B3O3H3 B3H3O6

B4C(S) B5H9 B10H14(L) B10H14 C(S) C CH CH2 CH2O CH3

CH4 CN CN2 C2 C2H C2H2 C2H4 C2N C2N2 C2O

C3 C3O2 C4 C5 HCN HNO HO2 H2O(S) H2O(L) H2O2

H3B3O6 N NH NH2 NH3 NO2 N2C N2H4 N2O N2O4

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

END

ESI-2: C* and I_{sp} of the HILs and UDMH with WFNA, RFNA, N_2O_4 and H_2O_2 oxidizers

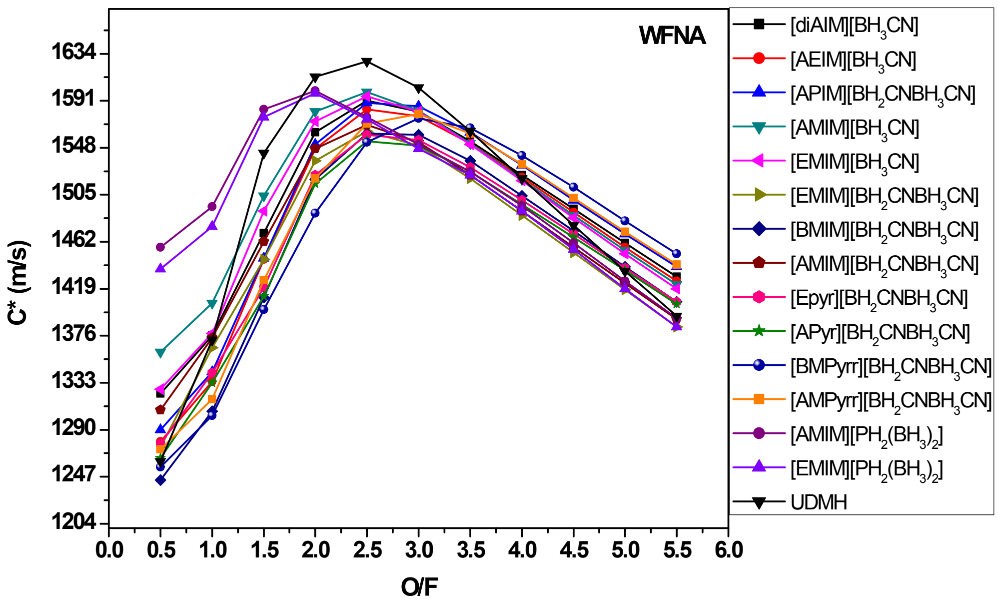

Figure SI-2a. C* of the HILs with WFNA at different O/F ($P_c = 2.4 \times 10^6$ Pa, $P_e = 9.8 \times 10^4$ Pa, $A_e/A_t = 4$).

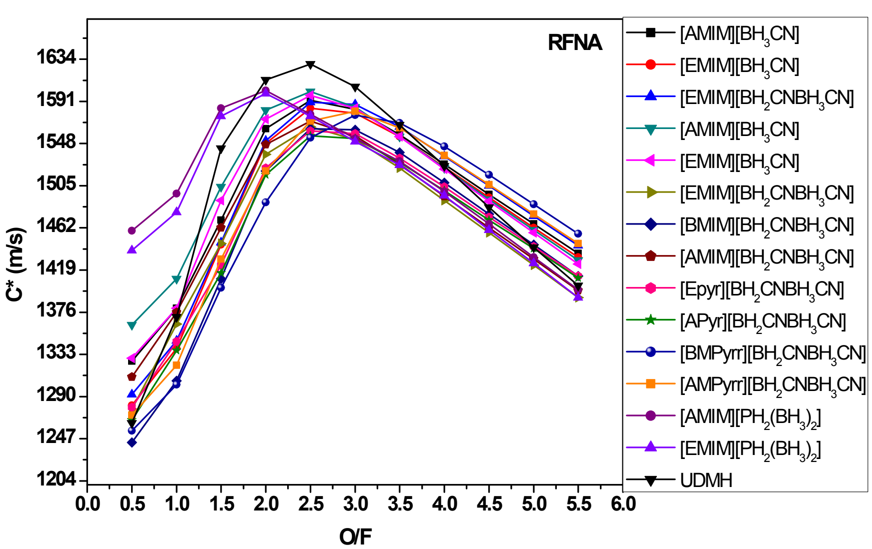

Figure SI-2b. C* of HILs with RFNA at different O/F ($P_c = 2.4 \times 10^6$ Pa, $P_e = 9.8 \times 10^4$ Pa, $A_e/A_t = 4$).

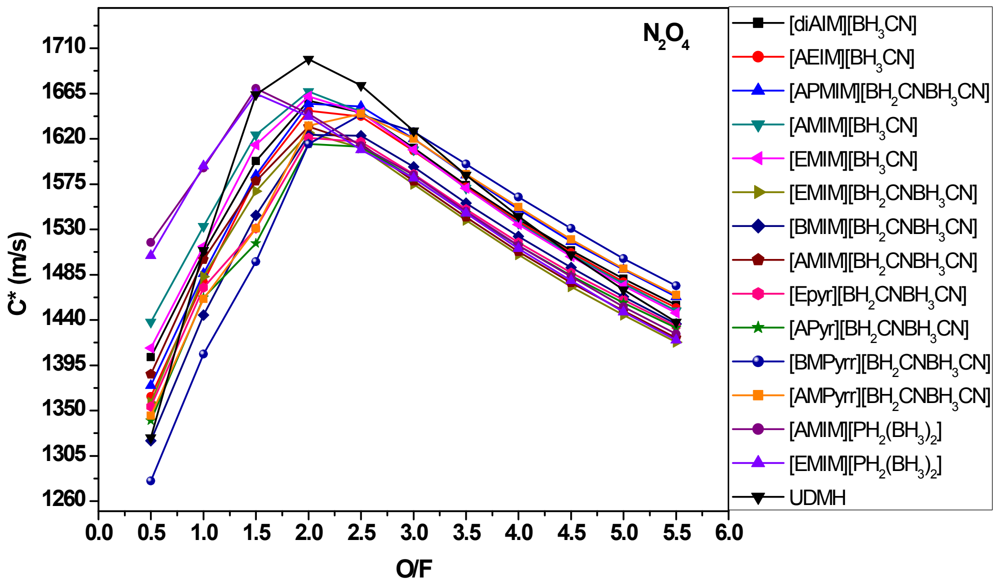

Figure SI-2c. C* of HILs with N_2O_4 at different O/F (P_c = 2.4 x 10^6 Pa, P_e= 9.8 x 10^4 Pa, A_e/A_t= 4).

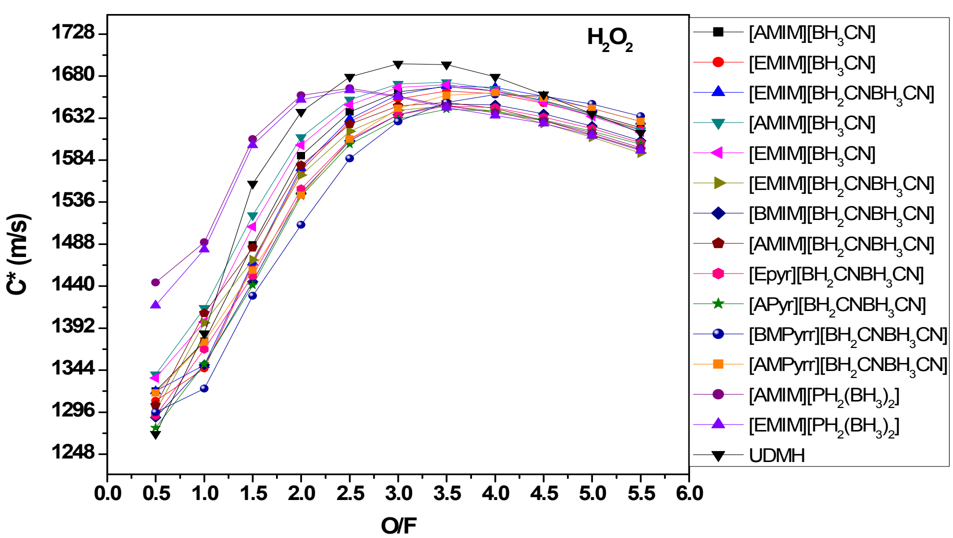

Figure SI-2d. C* of HILs with H_2O_2 at different O/F (P_c = 2.4 x 10^6 Pa, P_e= 9.8 x 10^4 Pa, A_e/A_t= 4).

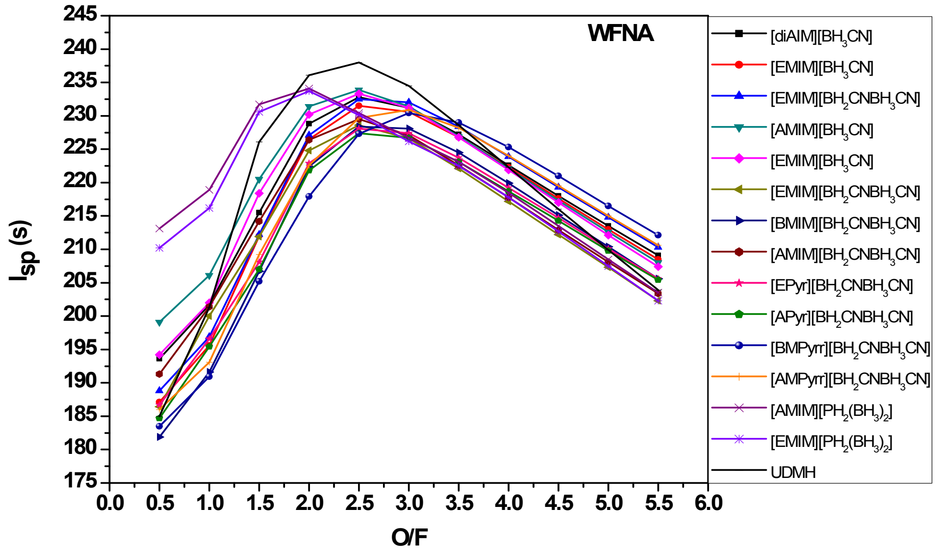

Figure SI-2e. I_{sp} of HILs with WFNA at different O/F (P_c = 2.4 x 10^6 Pa, P_e= 9.8 x 10^4 Pa, A_e/A_t= 4).

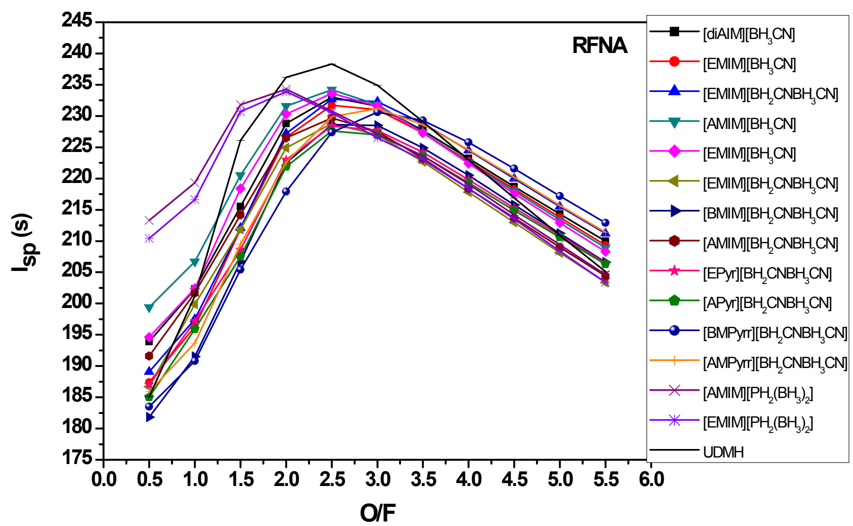

Figure SI-2f. I_{sp} of HILs with RFNA at different O/F (P_c = 2.4 x 10^6 Pa, P_e= 9.8 x 10^4 Pa, A_e/A_t= 4).

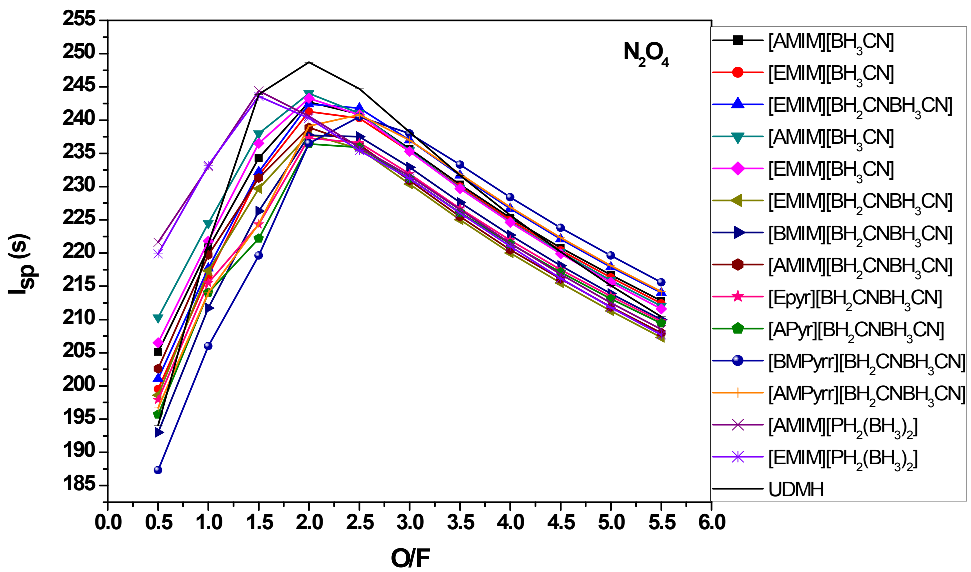

Figure SI-2g. I_{sp} of HILs with N_2O_4 at different O/F (Pc = 2.4 x 10^6 Pa, P_e= 9.8 x 10^4 Pa, A_e/A_t= 4).

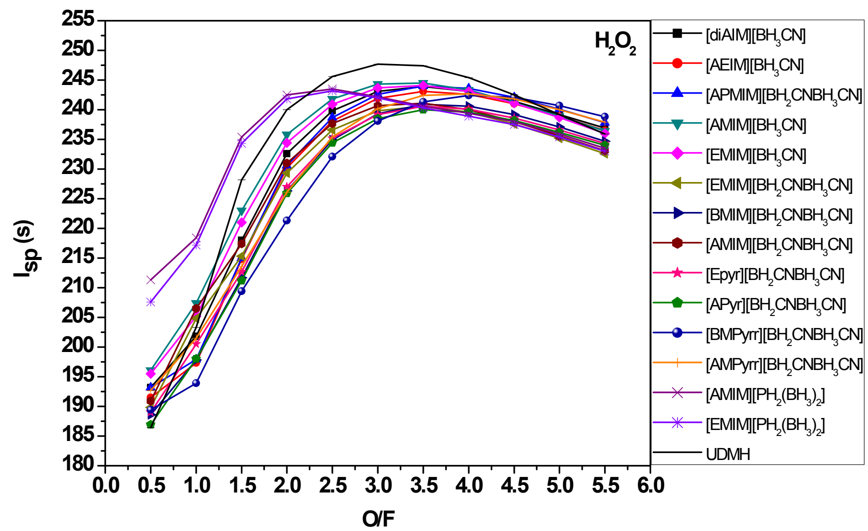

Figure SI-2h. I_{sp} of HILs with H_2O_2 at different O/F (P_c = 2.4 x 10^6 Pa, P_e= 9.8 x 10^4 Pa, A_e/A_t= 4).