Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting material

Can the sensitivity of energetic materials be tuned by using hydrogen bonds? Another look at the role of hydrogen bonding in the design of high energetic compounds.

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Table S1. Cartesian coordinates of optimized geometry of TNB molecule (M06/cc-PVDZ level of theory)

C	0.7030170000	1.2178130000	0.0000000000
C	-0.6848450000	1.1860330000	0.0000000000
C	-1.4064170000	0.0000000000	0.0000000000
C	1.3694200000	0.0000000000	0.0000000000
C	0.7030170000	-1.2178130000	0.0000000000
C	-0.6848450000	-1.1860330000	0.0000000000
N	-1.4283330000	2.4742530000	0.0000000000
O	-2.6473040000	2.4121000000	0.0000000000
O	-0.7647360000	3.4986750000	0.0000000000
N	-1.4283330000	-2.4742530000	0.0000000000
O	-0.7647360000	-3.4986750000	0.0000000000
O	-2.6473040000	-2.4121000000	0.0000000000
N	2.8567330000	0.0000000000	0.0000000000
O	3.4122640000	1.0868120000	0.0000000000
O	3.4122640000	-1.0868120000	0.0000000000
H	1.2434150000	2.1535370000	0.0000000000
H	-2.4869740000	0.0000000000	0.0000000000
H	1.2434150000	-2.1535370000	0.0000000000

Table S2. Cartesian coordinates of optimized geometry of TNP molecule (M06/cc-PVDZ level of theory)

O	-2.5820810000	0.0060580000	-0.0806600000
O	-0.4542640000	-3.5205200000	-0.0024420000
O	-0.8091850000	3.3670570000	-0.7032510000
O	-2.3842110000	-2.5431130000	-0.1023620000
O	-2.2123090000	2.5848710000	0.7650560000
O	3.6094110000	-1.0051200000	0.0587810000
O	3.5540420000	1.1681520000	0.0571550000
N	-1.1422240000	-2.5221050000	-0.0401290000
N	-1.2579690000	2.4857780000	0.0154800000
N	3.0232800000	0.0671350000	0.0480750000
C	-0.4887660000	-1.2114090000	-0.0131040000
C	-0.5395220000	1.1911460000	-0.0034060000
C	-1.2667530000	-0.0217370000	-0.0214880000
C	1.5468640000	0.0316940000	0.0223830000
C	0.9010570000	-1.1890810000	0.0182140000
C	0.8382220000	1.2308400000	-0.0031620000
H	1.4600350000	-2.1143050000	0.0313780000
H	1.3599230000	2.1782790000	-0.0212080000
H	-2.8994100000	-0.9274270000	-0.1089960000

Table S3. Cartesian coordinates of optimized geometry of TNT molecule (M06/cc-PVDZ level of theory)

O	0.6479200000	3.3861690000	-0.6967510000
O	0.6530260000	-3.3848880000	-0.6976800000
O	2.1686750000	2.6402540000	0.6653120000
O	2.1709830000	-2.6378340000	0.6669030000
O	-3.5922830000	1.0845910000	0.1272470000
O	-3.5911220000	-1.0887970000	0.1247410000
N	1.1692980000	2.5097710000	-0.0249740000
N	1.1723550000	-2.5082180000	-0.0246270000
N	-3.0347930000	-0.0017770000	0.1035060000
C	1.2741870000	0.0007590000	-0.0538940000
C	0.5079600000	1.1796110000	-0.0246180000
C	0.5093280000	-1.1789980000	-0.0243310000
C	-1.5535220000	-0.0009260000	0.0441420000
C	-0.8784630000	1.2075480000	0.0122110000
C	-0.8770480000	-1.2086140000	0.0124600000
C	2.7744680000	0.0012190000	-0.1834210000
H	-1.4166210000	2.1450230000	0.0130070000
H	-1.4141320000	-2.1467130000	0.0133160000
H	3.2411840000	-0.0000040000	0.8039580000
H	3.1212980000	-0.8845860000	-0.7116240000
H	3.1211870000	0.8882850000	-0.7094660000

Table S4. Cartesian coordinates of the geometry corresponding to the strongest N-O···H-O interaction in model system TNB/H_2O

C	0.7848890000	0.5090990000	-0.0135240000
C	0.5413350000	-0.8575930000	-0.0114470000
C	-0.7410290000	-1.3893810000	-0.0022960000
C	-0.3167160000	1.3538310000	-0.0060110000
C	-1.6220530000	0.8814220000	0.0032850000
C	-1.8027950000	-0.4949870000	0.0049230000
N	1.7007340000	-1.7892670000	-0.0193420000
O	1.4529820000	-2.9844110000	-0.0172820000
O	2.8145290000	-1.2900680000	-0.0273000000
N	-3.1894930000	-1.0328120000	0.0148090000
O	-4.1004130000	-0.2204160000	0.0209910000
O	-3.3144040000	-2.2469580000	0.0160120000
N	-0.0893660000	2.8236640000	-0.0080020000
O	1.0695650000	3.2065300000	-0.0162460000
O	-1.0784600000	3.5388010000	-0.0012450000
H	1.7921980000	0.9001060000	-0.0207050000
H	-0.9062030000	-2.4572390000	-0.0008500000
H	-2.4641520000	1.5585080000	0.0090200000
H	4.8676910000	-0.3698470000	-0.0419700000
O	5.7456240000	0.0236400000	-0.0482430000
H	5.9801830000	0.1260920000	0.8791850000

Table S5. Cartesian coordinates of the geometry corresponding to the strongest N-O···H-O interaction in model system TNP/H_2O

O	-2.5779410000	1.5092130000	-0.0643640000
O	-2.9476550000	-2.5927340000	0.0240600000
O	0.8317380000	3.1692800000	-0.7317170000
O	-3.9266170000	-0.6631040000	-0.0663140000
O	-0.7438490000	3.3707400000	0.7560450000
O	1.8171210000	-2.9686970000	0.0264830000
O	3.0580310000	-1.1837770000	0.0069730000
N	-2.9121470000	-1.3808350000	-0.0157260000
N	-0.0424250000	2.7252420000	-0.0014410000
N	1.9787360000	-1.7574710000	0.0121110000
C	-1.6096810000	-0.7106520000	-0.0058280000
C	-0.2292810000	1.2564100000	-0.0159980000
C	-1.5332510000	0.7087440000	-0.0171010000
C	0.7671900000	-0.9126400000	0.0003470000
C	-0.4756320000	-1.5148200000	0.0124720000
C	0.9049150000	0.4733470000	-0.0288060000
H	-0.5721330000	-2.5914380000	0.0283070000
H	1.8857210000	0.9285450000	-0.0596840000
H	-3.3863080000	0.9442970000	-0.0818680000
H	5.0006310000	-0.1511980000	-0.0022760000
O	5.8501650000	0.3003680000	-0.0063210000
H	6.0694290000	0.4285970000	0.9216430000

Table S6. Cartesian coordinates of the geometry corresponding to the strongest N-O···H-O interaction in model system TNT/H_2O

O	0.8757170000	3.1327510000	0.7110180000
O	-2.9565520000	-2.4493910000	0.6855480000
O	-0.7917320000	3.3778070000	-0.6615210000
O	-3.7776190000	-0.9744570000	-0.6836820000
O	3.0771370000	-1.1626360000	-0.1007430000
O	1.8474270000	-2.9546750000	-0.1067080000
N	-0.0455560000	2.7048960000	0.0332360000
N	-2.8850210000	-1.4324060000	0.0133290000
N	2.0029720000	-1.7435360000	-0.0840190000
C	-1.5507370000	0.6946560000	0.0518590000
C	-0.2520800000	1.2338290000	0.0310030000
C	-1.5866580000	-0.7108690000	0.0215230000
C	0.7812910000	-0.9053930000	-0.0320540000
C	0.9075020000	0.4730470000	0.0012110000
C	-0.4596540000	-1.5190960000	-0.0084560000
C	-2.7887630000	1.5431960000	0.1738890000
H	1.8813980000	0.9420550000	0.0067550000
H	-0.5470080000	-2.5965260000	-0.0102830000
H	-3.1681690000	1.8064370000	-0.8158060000
H	-3.5789700000	1.0084320000	0.6968990000
H	-2.5765630000	2.4707020000	0.7016470000
H	5.0121060000	-0.1162200000	-0.1308690000
O	5.8583030000	0.3413970000	-0.1440440000
H	6.1035850000	0.4398490000	0.7810400000

Table S7. Cartesian coordinates of the geometry corresponding to the strongest C-H···O interaction in model system TNB/H_2O

C	0.490364	0.848855	0.000000
C	-0.895911	0.817465	0.000000
C	-1.616110	-0.367696	0.000000
C	1.156153	-0.367696	0.000000
C	0.490364	-1.584247	0.000000
C	-0.895911	-1.552857	0.000000
N	-1.639337	2.099994	0.000000
O	-2.849035	2.029593	0.000000
O	-0.978788	3.115892	0.000000
N	-1.639337	-2.835386	0.000000
O	-0.978788	-3.851284	0.000000
O	-2.849035	-2.764985	0.000000
N	2.638320	-0.367696	0.000000
O	3.185044	0.713728	0.000000
O	3.185044	-1.449120	0.000000
H	1.037469	1.791557	0.000000
H	-2.705667	-0.367696	0.000000
H	1.037469	-2.526949	0.000000
O	2.242149	3.867309	0.000000
H	2.543382	4.386354	0.753779
H	2.543382	4.386354	-0.753779

Table S8. Cartesian coordinates of the geometry corresponding to the strongest C-H···O interaction in model system TNP/H_2O

O	1.8648990000	-2.0999590000	-0.0647280000
O	3.5476330000	1.6378590000	-0.0063710000
O	-2.0740840000	-2.4369670000	-0.4640880000
O	3.8423020000	-0.4907240000	-0.1059450000
O	-0.3805210000	-3.3323420000	0.5398730000
O	-0.7999970000	3.5584600000	0.0539730000
O	-2.5533750000	2.2915550000	0.0669210000
N	3.1241300000	0.5104560000	-0.0423360000
N	-0.9615490000	-2.4066630000	0.0218750000
N	-1.3549280000	2.4794640000	0.0512360000
C	1.6758520000	0.3034710000	-0.0113230000
C	-0.2766130000	-1.0961000000	0.0030710000
C	1.1376280000	-1.0137500000	-0.0141360000
C	-0.4947360000	1.2843630000	0.0270230000
C	0.8763910000	1.4375360000	0.0180620000
C	-1.0805610000	0.0241730000	0.0058000000
H	1.3291140000	2.4290240000	0.0270300000
H	-2.1654360000	-0.0836880000	-0.0098990000
H	2.8110060000	-1.8090110000	-0.1059570000
O	-4.5036650000	-0.3161610000	-0.0437360000
H	-5.0916070000	-0.3581460000	-0.8059000000
H	-5.1099590000	-0.3929110000	0.7011460000

Table S9. Cartesian coordinates of the geometry corresponding to the strongest C-H···O interaction in model system TNT/H_2O

O	3.481239	-1.616536	0.534766
O	-2.026667	2.449478	0.541447
O	3.815125	0.218165	-0.557047
O	-0.373462	3.310067	-0.552162
O	-0.856285	-3.548946	-0.106344
O	-2.596620	-2.264332	-0.104353
N	3.108134	-0.589418	0.009751
N	-0.936108	2.395976	0.014539
N	-1.401119	-2.465920	-0.086172
C	1.154363	0.995816	0.066537
C	1.649746	-0.320767	0.029611
C	-0.249816	1.081388	0.031834
C	-0.524306	-1.278141	-0.033868
C	0.847013	-1.450277	-0.006775
C	-1.092755	-0.018423	-0.004479
C	2.037801	2.192368	0.214388
H	1.285445	-2.448117	-0.010092
H	-2.175484	0.106573	-0.005996
H	2.323723	2.581217	-0.774856
H	1.522770	3.001740	0.742658
H	2.963683	1.938055	0.741139
O	-4.460307	0.370346	-0.009196
H	-5.060684	0.411819	0.743240
H	-5.052258	0.466522	-0.763302

Table S10. Comparison of energies of N-O···H-O and C-H···O-H interactions for TNB, TNP and TNT molecules calculated at M06/cc-PVDZ level of theory.

HEM	$E_{N\text{-}O\ldots H\text{-}O}$	$E_{C\text{-}H\ldots O\text{-}H}$	ΔE^a
TNB	-1.45	-1.76	0.31
TNP	-1.55	-1.76	0.21
TNT	-1.60	-1.91	0.31

a Interaction energies and energy differences (ΔE) are given in kcal/mol