Supporting Information

Weak interactions within nitryl halide heterodimers

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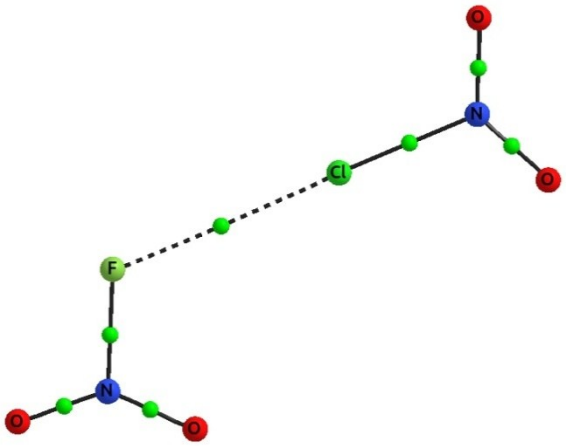
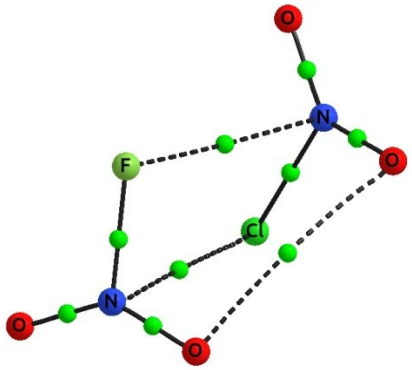
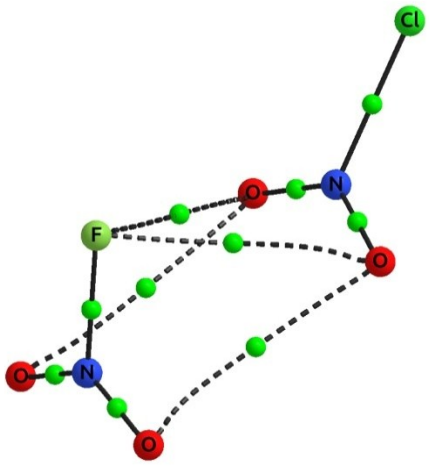
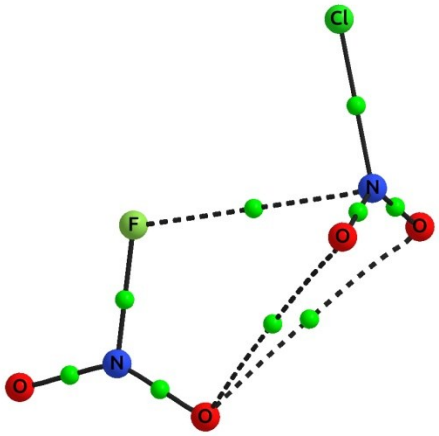
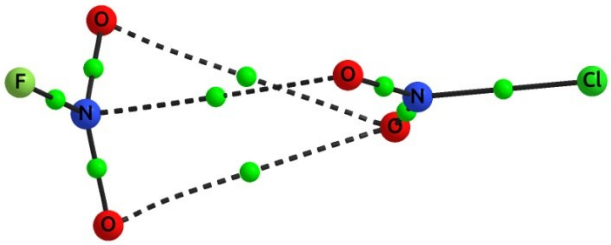
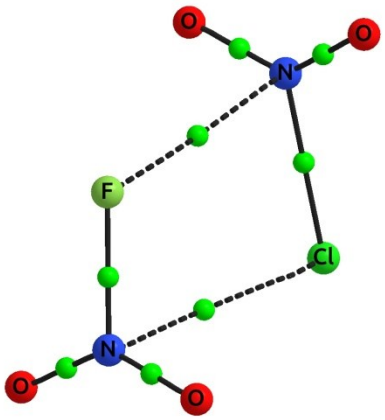
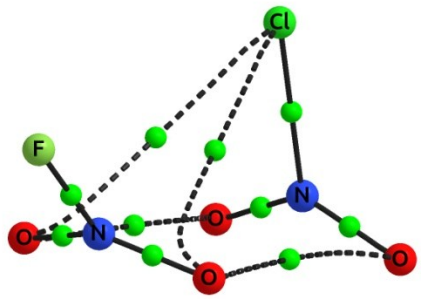
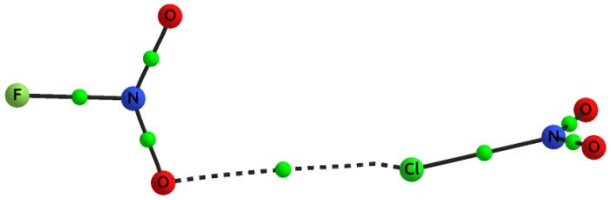
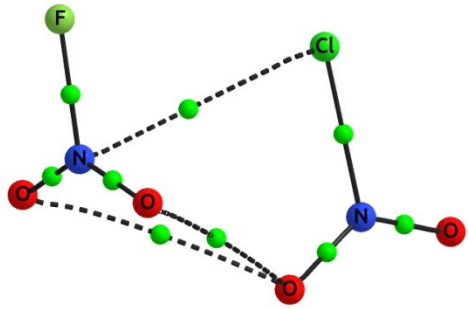
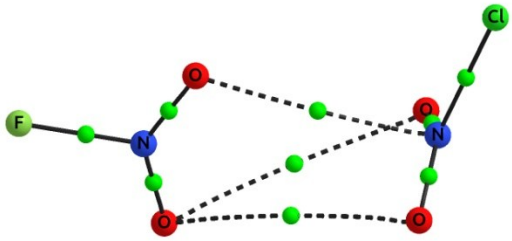
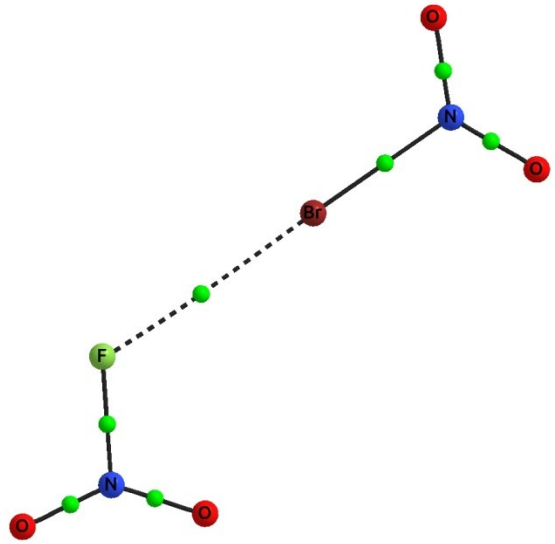
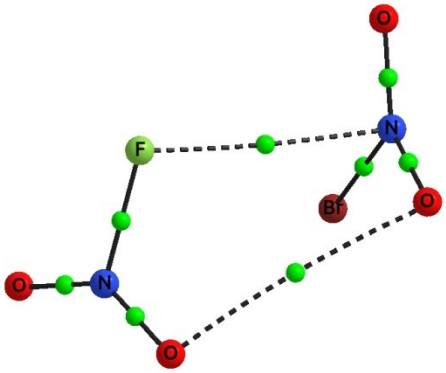
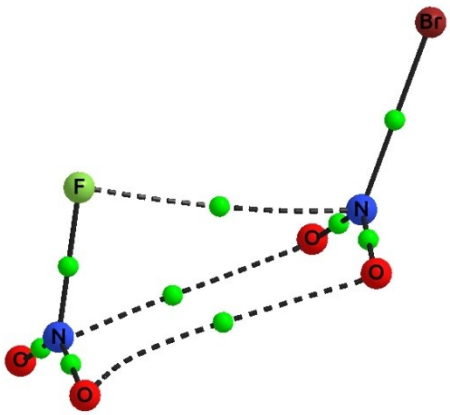
- **Table S1**. AIM molecular graphs and Cartesian coordinates of all complexes studied at scs-MP2/aug-cc-pVTZ computational level.
- **Table S2.** Interatomic interaction distances (Å) for all the complexes studied.
- **Table S3.** Electron density (ρ_{BCP}) and Laplacian ($\nabla^2\rho_{BCP}$) in a.u. at MP2/aug-cc-pVTZ computational level.
- **Table S5.** Total NBO charge (in a.u.) of monomer NO_2X in the complexes at MP2/aug-cc-pVTZ computational level.

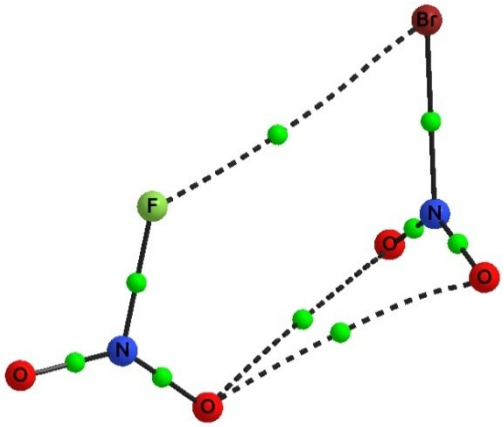
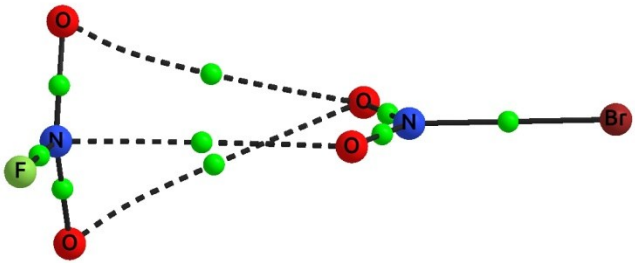
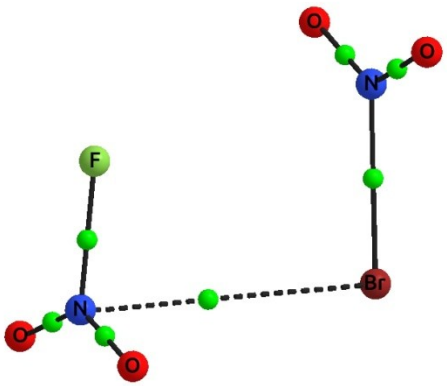
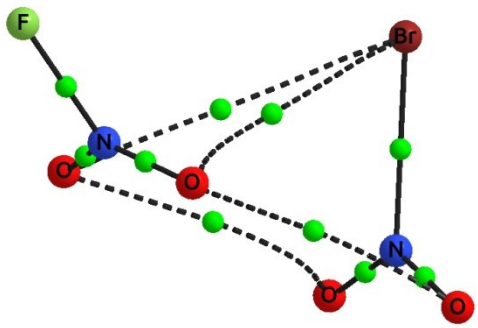
Table S1. AIM molecular graphs and Cartesian coordinates of all complexes studied at scs-MP2/aug-cc-pVTZ computational level.

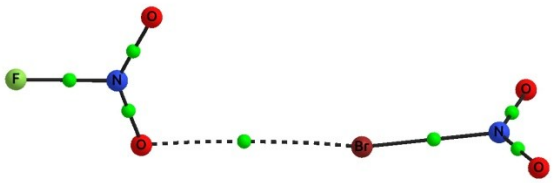
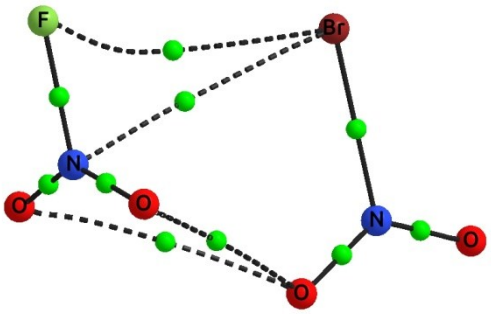
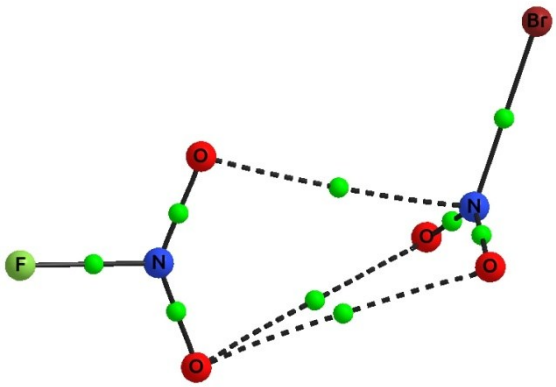
FCl_{1a} 	N -0.214748 2.914181 0.000000 O 0.134566 4.038796 0.000000 O -1.228568 2.314881 0.000000 Cl 0.302541 -0.999143 0.000000 N -0.114345 -2.810661 0.000000 O 0.841688 -3.531746 0.000000 O -1.289930 -3.040379 0.000000 F 0.976846 1.972149 0.000000
FCl_{2a} 	N 1.599650 0.052836 -0.439563 Cl 1.067552 0.063316 1.394888 O 2.025013 -0.999066 -0.797108 O 1.438369 1.103973 -0.975818 N -1.911159 0.062131 -0.078284 O -2.456949 -0.612841 0.714753 O -1.824427 1.203644 -0.350327 F -1.073631 -0.788803 -1.035060
FCl_{3a} 	N -0.495049 -1.152370 0.000000 O -0.726623 -0.722645 -1.093433 O -0.726623 -0.722645 1.093433 N 0.060530 2.260673 0.000000 O -0.284708 2.503877 -1.099025 O -0.284708 2.503877 1.099025 F 1.303227 1.383257 0.000000 Cl 0.386098 -2.786806 0.000000
FCl_{4a} N/A	N/A
FCl_{5a}	N -2.225441 -0.063477 0.000000 O -1.890486 1.066231 0.000000 O -3.229272 -0.677687 0.000000

	N 1.283678 0.685696 0.000000 O 1.020846 1.091468 1.093190 O 1.020846 1.091468 -1.093190 F -1.017300 -0.986032 0.000000 Cl 2.306301 -0.877904 0.000000
FCl_{6a} 	N -2.208278 -0.229335 0.000000 O -2.026017 -0.619862 1.097534 O -2.026017 -0.619862 -1.097534 N 1.233790 -0.097044 0.000000 O 0.953644 -1.261459 0.000000 O 0.550155 0.887576 0.000000 Cl 3.055235 0.249131 0.000000 F -2.836959 1.134611 0.000000
FCl_{1b} N/A	N/A
FCl_{2b} 	N 0.400170 -1.681593 0.000000 O 0.833808 -1.848328 -1.095310 O 0.833808 -1.848328 1.095310 N 0.069728 1.968859 0.000000 O -0.262099 2.223031 -1.099208 O -0.262099 2.223031 1.099208 F 1.288856 1.043728 0.000000 Cl -1.392320 -1.010997 0.000000
FCl_{3b} 	N -0.390984 -1.699378 0.000000 O -0.669902 -1.362967 -1.097239 O -0.669902 -1.362967 1.097239 N -0.403987 1.703422 0.000000 O -0.850415 1.860103 -1.095325 O -0.850415 1.860103 1.095325 F 0.569647 -2.840198 0.000000 Cl 1.381008 1.071694 0.000000

FCl_{4b} 	N 2.850565 0.126892 0.000000 O 3.305098 0.281161 1.094322 O 3.305098 0.281161 -1.094322 Cl 1.074027 -0.475463 0.000000 N -2.602101 0.109699 0.000000 O -2.244716 1.233589 0.000000 O -2.098248 -0.957901 0.000000 F -4.096766 0.007110 0.000000
FCl_{5b} 	N -1.860586 0.436956 0.000000 O -1.064623 1.330348 0.000000 O -3.054265 0.416848 0.000000 Cl -1.068202 -1.262409 0.000000 N 1.917959 0.380313 0.000000 O 1.771545 0.783226 1.098020 O 1.771545 0.783226 -1.098020 F 2.435983 -1.037321 0.000000
FCl_{6b} 	N -1.393110 -0.637296 0.000000 O -1.099942 -1.022293 1.093697 O -1.099942 -1.022293 -1.093697 N 2.012128 0.078006 0.000000 O 2.086114 -1.099264 0.000000 O 1.150409 0.886481 0.000000 F 3.362100 0.718855 0.000000 Cl -2.514048 0.854462 0.000000
FBr_{1a}	N -0.248828 3.255088 0.000000 O 0.183253 4.349310 0.000000 O -1.300403 2.726849 0.000000 N -0.200728 -2.719038 0.000000 O 0.764654 -3.434312 0.000000 O -1.373686 -2.980561 0.000000 F 0.879963 2.223631 0.000000 Br 0.215205 -0.755032 0.000000

	
FBr_{2a} 	N 1.081962 0.059104 -1.152066 O 1.401566 -0.972575 -1.660860 O 0.735267 1.111707 -1.599270 N -2.268594 0.069872 0.108387 O -2.664754 -0.546030 1.028915 O -2.208575 1.193855 -0.235567 F -1.657083 -0.853537 -0.943455 Br 1.149871 0.022757 0.901146
FBr_{3a} 	N -0.797306 -0.401243 0.000000 O -1.060689 0.022529 -1.092575 O -1.060689 0.022529 1.092575 N 0.200636 2.829674 0.000000 O -0.097327 3.126930 -1.099295 O -0.097327 3.126930 1.099295 F 1.278152 1.750438 0.000000 Br 0.264421 -2.103001 0.000000
FBr_{4a} N/A	N/A
FBr_{5a}	N -2.828885 -0.164735 0.000000 O -2.459887 0.955459 0.000000 O -3.854354 -0.743231 0.000000 N 0.702108 1.108553 0.000000 O 0.422366 1.513787 1.093041 O 0.422366 1.513787 -1.093041

	F -1.656757 -1.121976 0.000000 Br 1.861789 -0.547359 0.000000
FBr_{6a} 	N -2.991831 -0.195804 0.000000 O -2.849317 -0.602222 1.097620 O -2.849317 -0.602222 -1.097620 N 0.450956 -0.191978 0.000000 O 0.128243 -1.348728 0.000000 O -0.213535 0.809528 0.000000 F -3.486573 1.222184 0.000000 Br 2.432366 0.126510 0.000000
FBr_{1b} N/A	N/A
FBr_{2b} 	N 1.006579 -1.489338 0.000000 O 1.468791 -1.618516 -1.094437 O 1.468791 -1.618516 1.094437 N 0.041771 2.387660 0.000000 O -0.348368 2.551598 -1.098766 O -0.348368 2.551598 1.098766 F 1.441892 1.801451 0.000000 Br -0.975231 -0.959400 0.000000
FBr_{3b} 	N -0.288894 -2.183157 0.000000 O -0.599947 -1.878773 -1.097593 O -0.599947 -1.878773 1.097593 N -1.103991 1.256224 0.000000 O -1.588324 1.275617 -1.094468 O -1.588324 1.275617 1.094468 F 0.783841 -3.223948 0.000000

	Br 0.934063 1.170499 0.000000
FBr_{4b} 	N 2.762753 0.256670 0.000000 O 3.233081 0.397938 1.093597 O 3.233081 0.397938 -1.093597 N -2.979561 0.183119 0.000000 O -2.715574 1.332724 0.000000 O -2.386398 -0.838715 0.000000 F -4.455614 -0.044942 0.000000 Br 0.824189 -0.324664 0.000000
FBr_{5b} 	N -1.479590 1.040754 0.000000 O -0.523284 1.766461 0.000000 O -2.654514 1.272498 0.000000 N 2.289864 0.392738 0.000000 O 2.196788 0.810110 1.098055 O 2.196788 0.810110 -1.098055 F 2.621490 -1.081485 0.000000 Br -1.008711 -0.927005 0.000000
FBr_{6b} 	N -0.624703 -0.950226 0.000000 O -0.266618 -1.290150 1.092986 O -0.266618 -1.290150 -1.092986 N 2.623940 0.180771 0.000000 O 2.750196 -0.991778 0.000000 O 1.728100 0.950796 0.000000 F 3.946595 0.882016 0.000000 Br -2.078618 0.450007 0.000000
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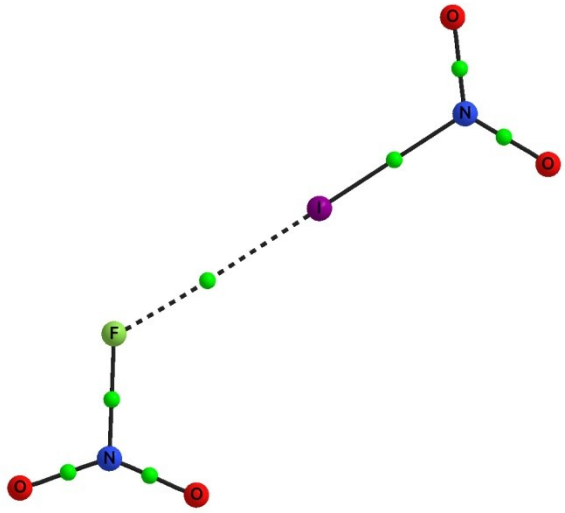
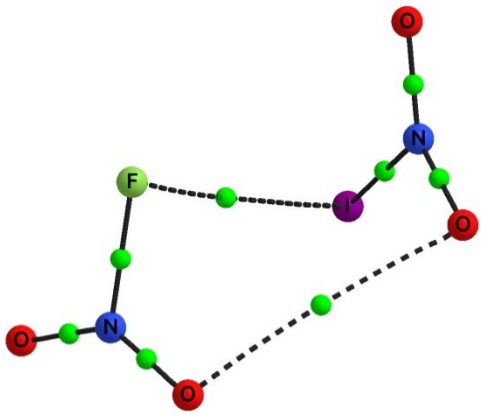
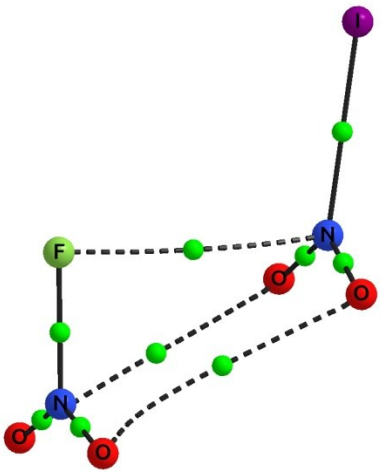
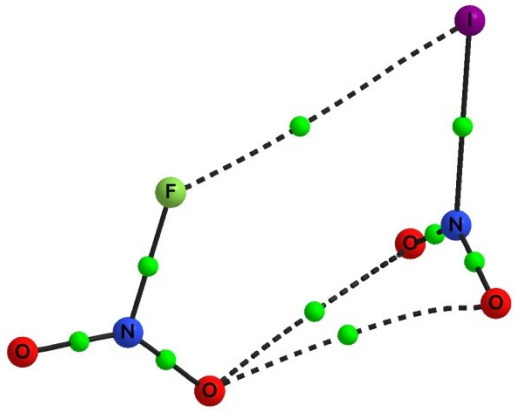
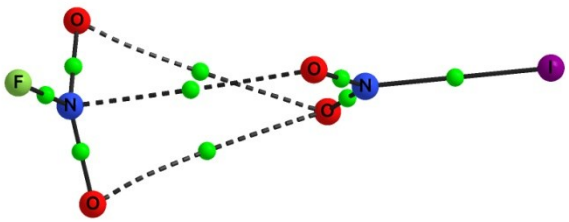
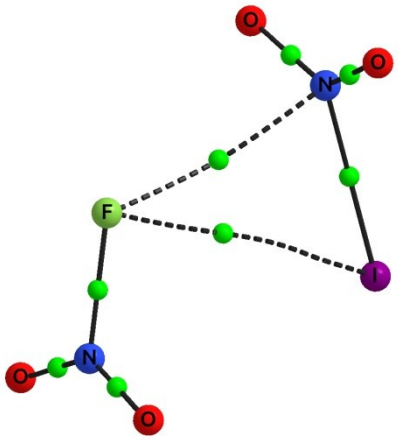
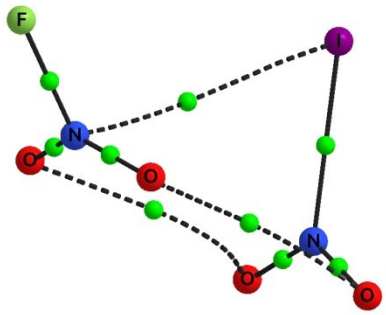
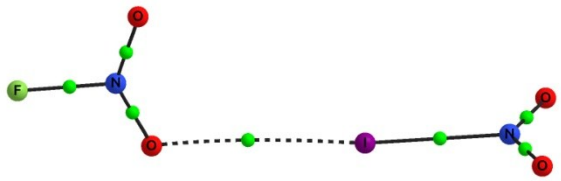
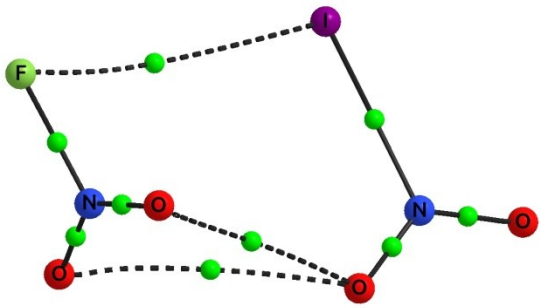
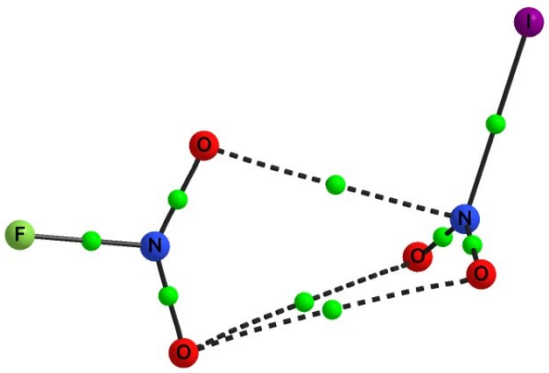
	I 0.162775 -0.574998 0.000000
FI_{2a} 	N 0.610451 0.054111 -1.544148 O 0.823037 -0.976776 -2.126452 O 0.183410 1.105387 -1.948321 N -2.574651 0.082479 0.306622 O -2.792243 -0.367962 1.372085 O -2.612090 1.133827 -0.222994 F -2.115485 -0.997824 -0.660068 I 1.087959 0.021535 0.604260
FI_{3a} 	N -0.929022 0.139272 0.000000 O -1.192656 0.589086 -1.090689 O -1.192656 0.589086 1.090689 N 0.281958 3.225996 0.000000 O 0.010677 3.545921 -1.099425 O 0.010677 3.545921 1.099425 F 1.268208 2.058339 0.000000 I 0.179594 -1.722221 0.000000
FI_{4a} N/A	N/A
FI_{5a}	N -3.202252 -0.277405 0.000000 O -2.896762 0.860881 0.000000 O -4.190931 -0.916261 0.000000 N 0.167674 1.310755 0.000000

	O -0.159603 1.709266 1.091453 O -0.159603 1.709266 -1.091453 F -1.972688 -1.167814 0.000000 I 1.564082 -0.363232 0.000000
FI_{6a} 	N -3.555613 -0.187709 0.000000 O -3.360304 -0.569276 1.097637 O -3.360304 -0.569276 -1.097637 N -0.107303 -0.207608 0.000000 O -0.480799 -1.356863 0.000000 O -0.766549 0.806634 0.000000 F -4.240331 1.155511 0.000000 I 2.043650 0.083557 0.000000
FI_{1b} N/A	N/A
FI_{2b} 	N 1.528365 -0.815447 0.000000 O 2.029085 -0.773180 -1.092663 O 2.029085 -0.773180 1.092663 N -0.245909 2.624097 0.000000 O -0.642458 2.768914 -1.098877 O -0.642458 2.768914 1.098877 F 1.182753 2.104724 0.000000 I -0.668251 -1.017940 0.000000
FI_{3b}	N -0.118768 -2.507996 0.000000 O -0.499322 -2.299679 -1.097723 O -0.499322 -2.299679 1.097723 N -1.524410 0.722670 0.000000 O -2.025358 0.633883 -1.092725 O -2.025358 0.633883 1.092725 F 1.200640 -3.217791 0.000000

	I 0.638215 1.098806 0.000000
FI_{4b} 	N 2.752159 0.273367 0.000000 O 3.255732 0.388272 1.091861 O 3.255732 0.388272 -1.091861 N -3.212662 0.214776 0.000000 O -3.043352 1.382417 0.000000 O -2.530523 -0.752764 0.000000 F -4.653202 -0.139213 0.000000 I 0.629237 -0.210323 0.000000
FI_{5b} 	N -1.072078 1.483815 0.000000 O -0.000558 2.043173 0.000000 O -2.182932 1.952253 0.000000 N 2.626504 0.287579 0.000000 O 2.591413 0.711554 1.098314 O 2.591413 0.711554 -1.098314 F 2.754593 -1.223284 0.000000 I -0.962088 -0.695520 0.000000
FI_{6b} 	N -0.110986 -1.172657 0.000000 O 0.266264 -1.524946 1.091461 O 0.266264 -1.524946 -1.091461 N 3.014785 0.245807 0.000000 O 3.260414 -0.907140 0.000000 O 2.046168 0.921764 0.000000 F 4.261576 1.080173 0.000000 I -1.694651 0.323260 0.000000
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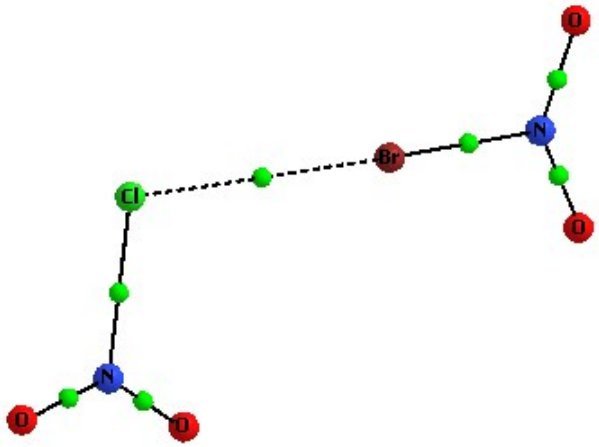
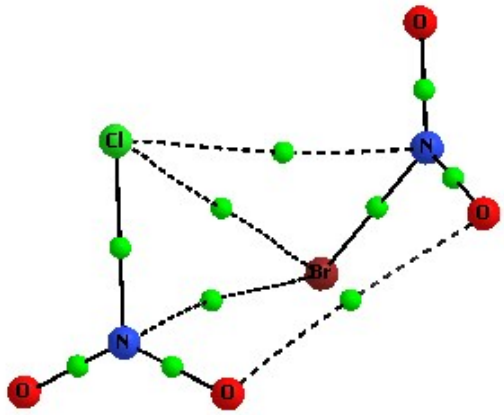
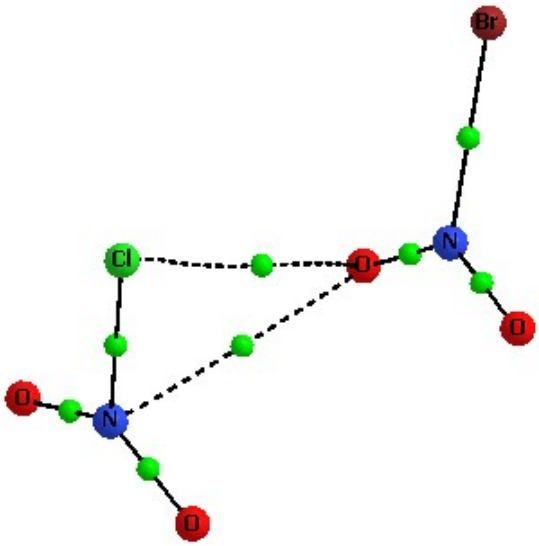
	Br 1.1734 -0.4747 0.0000 N 3.1131 0.0803 0.0000 O 3.8909 -0.8339 0.0000 O 3.2881 1.2680 0.0000 Cl -2.1422 -1.5033 0.0000
$ClBr_{2a}$ 	N 1.8081 0.1061 0.4792 Br 0.6572 -0.7881 1.9081 O 2.5981 -0.6290 -0.0364 O 1.5623 1.2664 0.3188 N -1.8011 0.1151 -0.5119 O -2.6268 -0.6203 -0.0654 O -1.5525 1.2690 -0.3369 Cl -0.6454 -0.7192 -1.7554
$ClBr_{3a}$ 	N 0.6454 -1.4315 0.4087 O -0.0552 -1.3723 -0.5658 O 0.3837 -1.3534 1.5759 N -1.1205 1.4018 -0.3902 O -1.4555 1.4237 -1.5340 O -1.6827 1.1173 0.6229 Br 2.6005 -1.7052 0.0057 Cl 0.6843 1.9197 -0.1232
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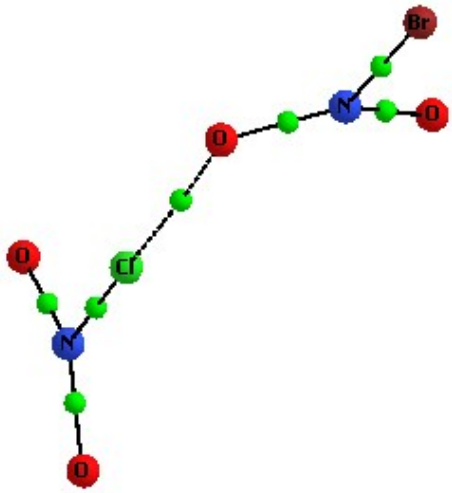
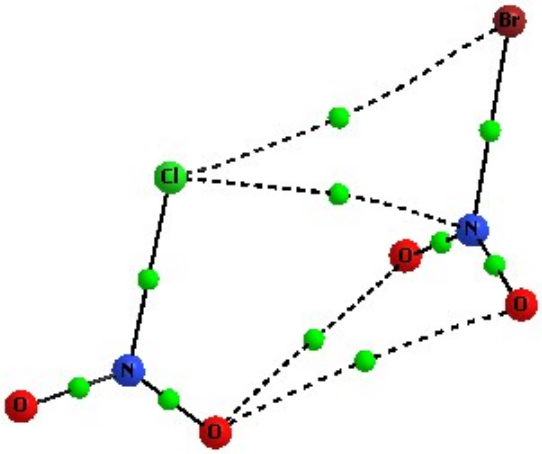
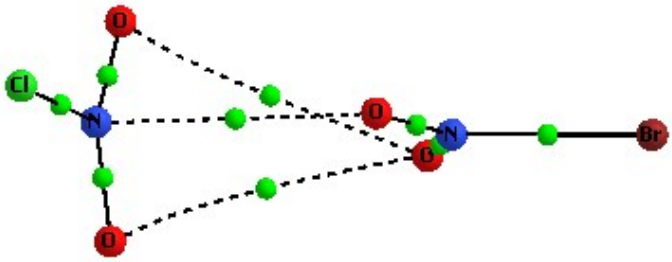
	O -1.7458 1.7668 0.0000 O -2.0810 -0.3942 0.0000 Br -4.3931 1.0669 0.0000 Cl 1.0223 -0.6533 0.0000
$ClBr_{5a}$ 	N -0.2913 2.0378 0.0000 O -1.1897 1.2501 0.0000 O -0.2539 3.2303 0.0000 N -0.1625 -1.8307 0.0000 O -0.6116 -1.6416 -1.0936 O -0.6116 -1.6416 1.0936 Br 1.7099 -2.6295 0.0000 Cl 1.4106 1.2251 0.0000
$ClBr_{6a}$ 	N -1.8061 -0.2950 0.0000 O -1.6010 -0.7295 1.0938 O -1.6010 -0.7295 -1.0938 N 1.6568 0.0184 0.0000 O 1.4668 -1.1661 0.0000 O 0.8884 0.9415 0.0000 Br 3.5979 0.5577 0.0000 Cl -2.6018 1.4027 0.0000
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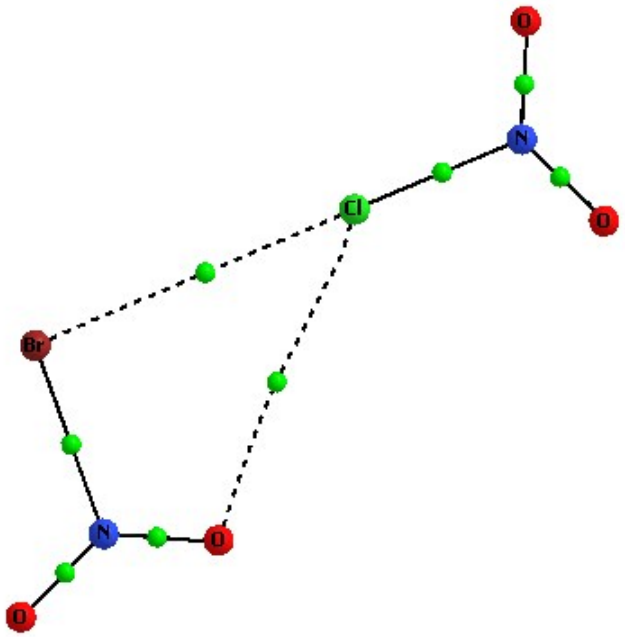
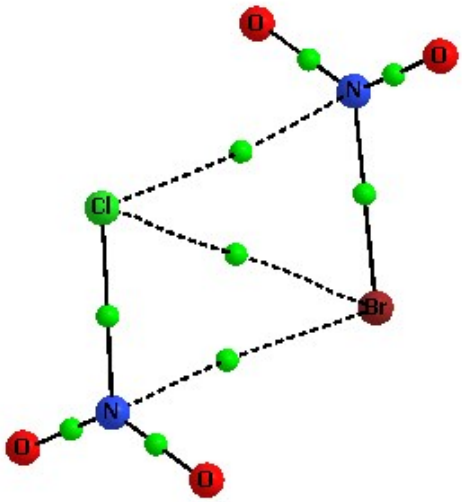
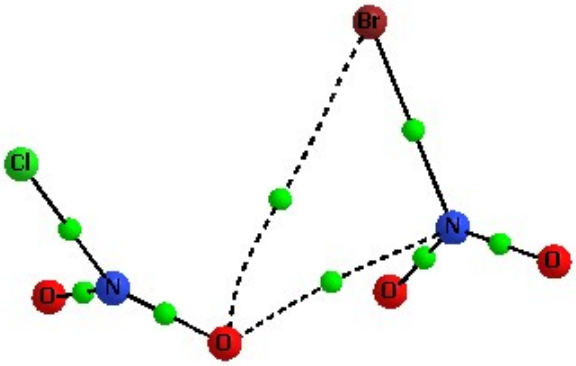
	Cl 1.1715 -0.6418 0.0000
$ClBr_{2b}$ 	N 0.7806 -1.8710 0.0000 O 1.2614 -1.9262 -1.0942 O 1.2614 -1.9262 1.0942 N -0.7457 1.8844 0.0000 O -1.2115 1.9724 -1.0948 O -1.2115 1.9724 1.0948 Br -1.2448 -1.6437 0.0000 Cl 1.1101 1.5378 0.0000
$ClBr_{3b}$ 	N -1.1237 -2.7617 0.8917 O -1.8128 -2.7095 -0.0866 O -1.3758 -2.6768 2.0569 N -3.0043 0.0473 0.0757 O -3.3617 0.0401 -1.0655 O -3.5468 -0.2746 1.0928 Br -1.0971 0.7329 0.3434 Cl 0.6873 -3.0202 0.5226
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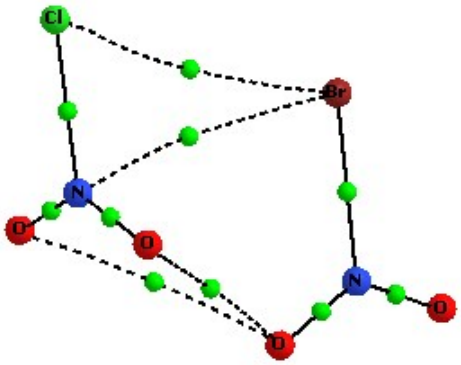
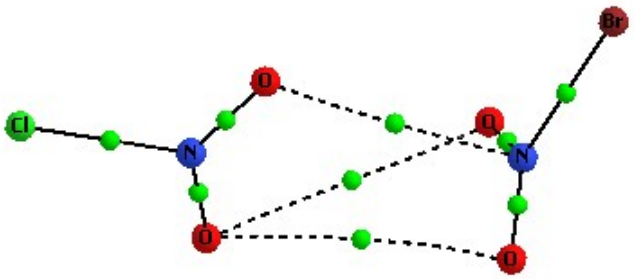
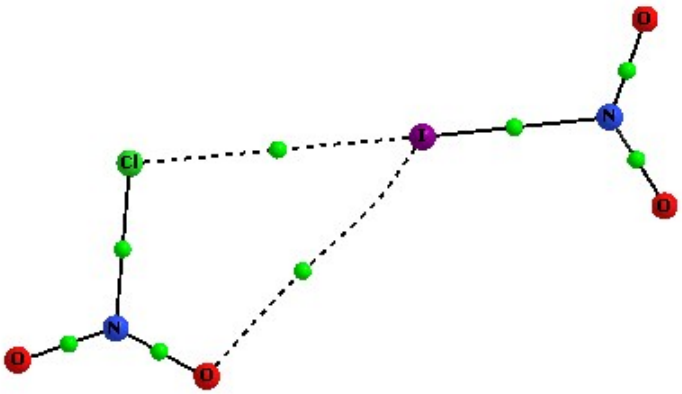
$ClBr_{5b}$ 	N -0.3669 2.0440 0.0000 O -1.2013 1.1832 0.0000 O -0.4480 3.2381 0.0000 N -0.0963 -1.8602 0.0000 O -0.5376 -1.6806 -1.0944 O -0.5376 -1.6806 1.0944 Br 1.5383 1.3343 0.0000 Cl 1.6493 -2.5782 0.0000
$ClBr_{6b}$ 	N -1.7104 -0.5945 0.0000 O -1.4190 -0.9893 1.0932 O -1.4190 -0.9893 -1.0932 N 1.6620 0.2883 0.0000 O 1.6784 -0.9075 0.0000 O 0.7624 1.0785 0.0000 Br -2.9081 1.0389 0.0000 Cl 3.3537 1.0748 0.0000
ClI_{1a} 	N -0.226382 -3.316559 0.000000 O -0.579295 -4.452565 0.000000 O 0.833387 -2.776244 0.000000 N 1.059170 2.759324 0.000000 O 0.361083 3.747250 0.000000 O 2.266572 2.681873 0.000000 Cl -1.699028 -2.079127 0.000000 I 0.000000 0.861194 0.000000
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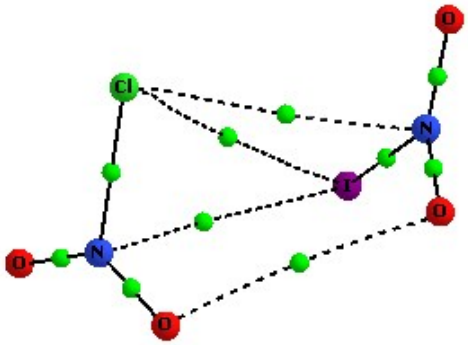
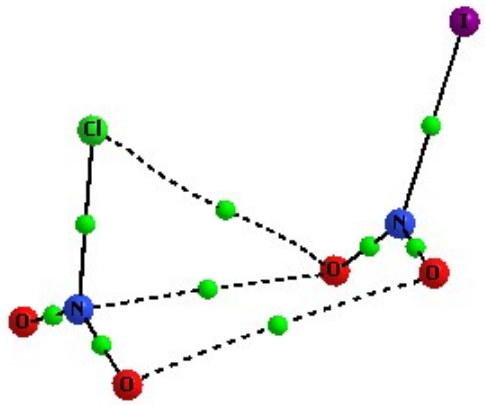
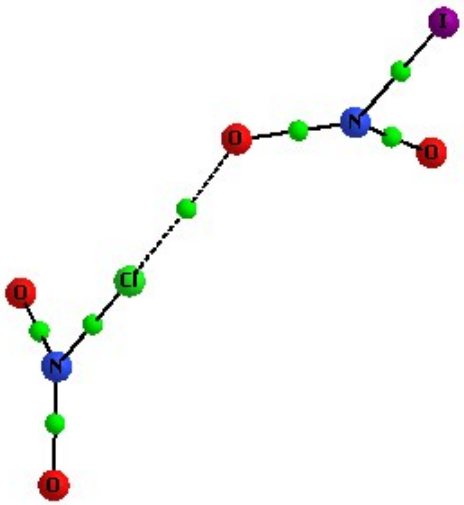
	O -2.494540 -1.643714 -0.135284 O -2.160122 -0.196292 1.473920 Cl -2.264491 0.828817 -0.915533 I 1.366847 -0.679976 -0.113191
ClI_{3a} 	N 0.278863 1.102216 -0.046601 O -0.368235 1.208806 0.970033 O 0.111909 1.635034 -1.116366 N -2.948100 0.050998 0.148185 O -3.296770 -0.070179 1.280861 O -3.088467 0.908442 -0.668024 I 1.980292 -0.247582 0.075005 Cl -1.949313 -1.435733 -0.495200
ClI_{4a} 	N 1.059948 -4.598631 0.000000 O 1.232904 -5.056122 1.093615 O 1.232904 -5.056122 -1.093615 N 0.031482 0.805803 0.000000 O 1.232904 0.687046 0.000000 O -0.822501 -0.049946 0.000000 Cl 0.404708 -2.863298 0.000000 I -0.708108 2.849566 0.000000
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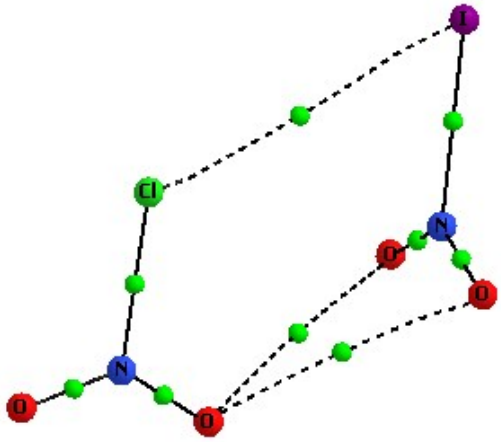
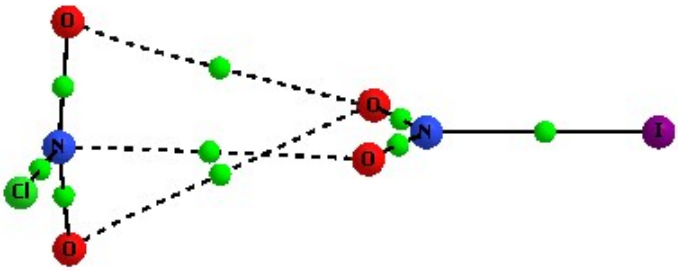
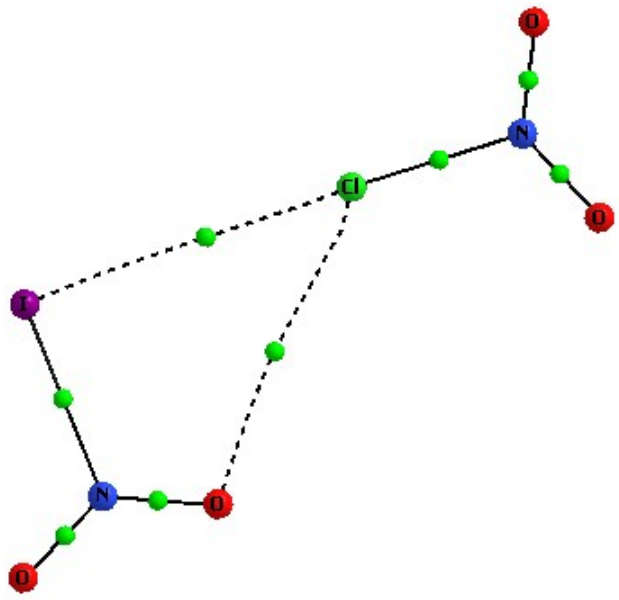
	
ClI_{6a} 	N 3.060777 -0.699250 0.000000 O 3.060777 -0.220575 1.093854 O 3.060777 -0.220575 -1.093854 N -0.221654 0.455962 0.000000 O 0.473295 1.443532 0.000000 O 0.106103 -0.707651 0.000000 Cl 3.059480 -2.578606 0.000000 I -2.367786 0.814745 0.000000
ClI_{1b} 	N 2.088314 1.095852 0.000000 O 2.910550 1.976806 0.000000 O 2.230797 -0.100047 0.000000 N -1.546915 -3.510623 0.000000 O -2.727841 -3.700931 0.000000 O -0.610854 -4.255203 0.000000 Cl -1.071236 -1.697892 0.000000 I 0.000000 1.781180 0.000000
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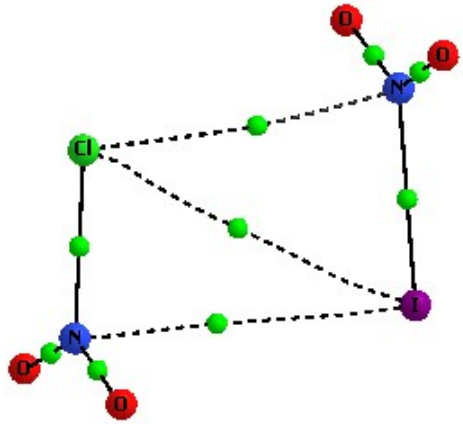
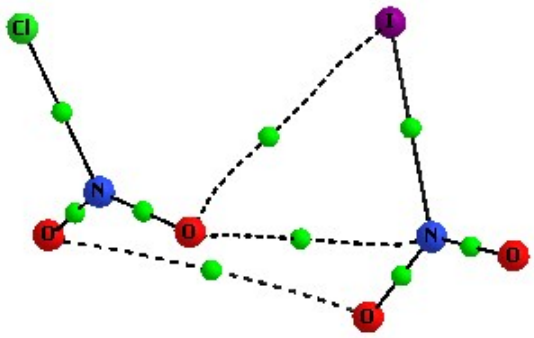
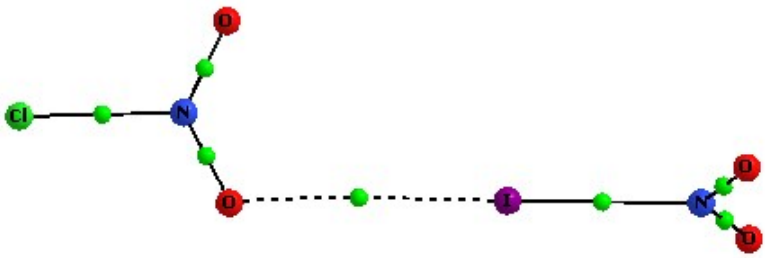
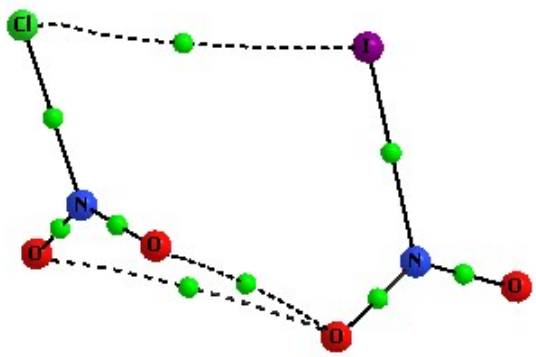
	O -0.738340 2.615198 -1.094542 Cl -2.398959 0.943581 0.000000 I 1.401499 -0.502363 0.000000
ClI_{3b} 	N -2.134915 0.658020 0.136927 O -1.660100 1.259366 -0.782515 O -2.166113 0.873690 1.311293 N 1.300751 1.343594 -0.112168 O 1.627779 1.752944 -1.196308 O 0.989147 1.944928 0.884865 I 1.251570 -0.845684 0.081235 Cl -2.989397 -0.931616 -0.36573
ClI_{4b} 	N -0.157455 3.135372 0.000000 O -0.240625 3.650488 1.091455 O -0.240625 3.650488 -1.091455 N -0.240625 -2.753624 0.000000 O -1.405119 -2.475109 0.000000 O 0.743024 -2.062535 0.000000 Cl 0.118224 -4.559662 0.000000 I 0.187236 0.995007 0.000000
ClI_{5b} 	N 1.172817 1.736139 0.000000 O 1.988279 0.846187 0.000000 O 1.331591 2.930480 0.000000 N 0.899654 -2.212743 0.000000 O 1.331591 -2.018695 1.094648 O 1.331591 -2.018695 -1.094648 Cl -0.825913 -2.996694 0.000000 I -0.911909 1.063506 0.000000
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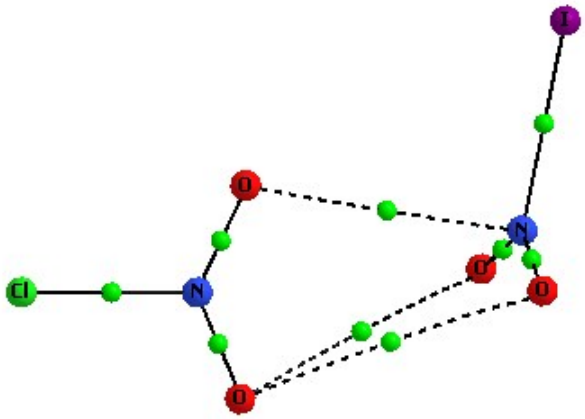
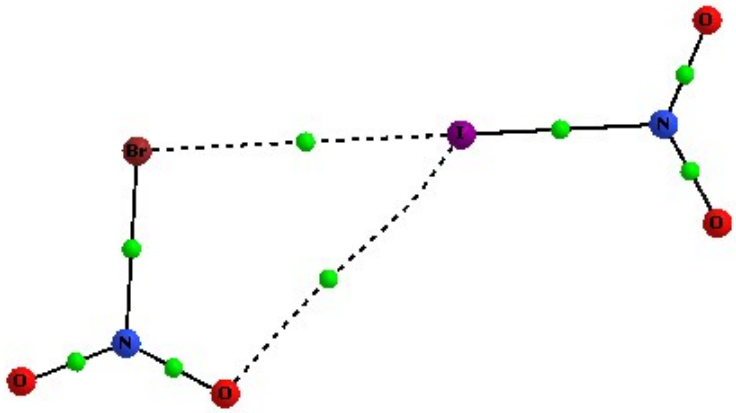
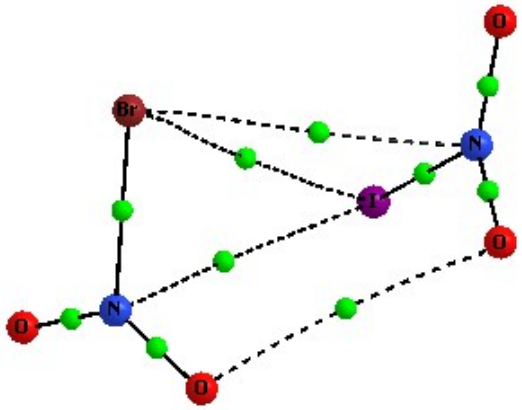
	O -0.772807 1.456515 -1.091583 N -1.965171 -1.666032 0.000000 O -2.841926 -0.854284 0.000000 O -0.772807 -1.563348 0.000000 Cl -2.565412 -3.438850 0.000000 I 1.896279 1.065554 0.000000
BrI_{1a} 	N 0.656757 -2.998789 0.000000 O 0.591745 -4.190557 0.000000 O 1.568760 -2.229548 0.000000 N 0.747967 3.231250 0.000000 O -0.096792 4.097351 0.000000 O 1.952634 3.345131 0.000000 I 0.000000 1.188218 0.000000 Br -1.198967 -2.079480 0.000000
BrI_{2a} 	N 1.148884 1.391659 0.528007 O 1.226875 2.308356 -0.249967 O 0.781576 1.376691 1.676108 N -1.826489 -1.046904 0.602373 O -1.894672 -2.086224 0.012275 O -1.571313 -0.785910 1.742941 I 1.770902 -0.554473 -0.266680 Br -2.212980 0.584871 -0.549413
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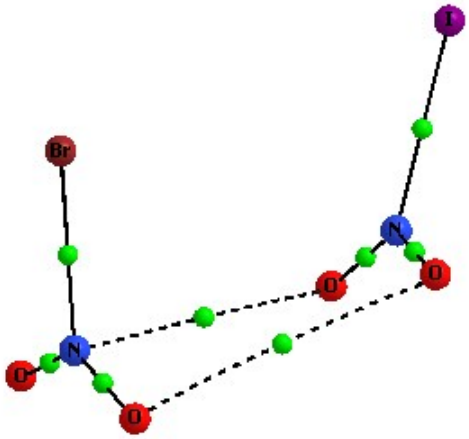
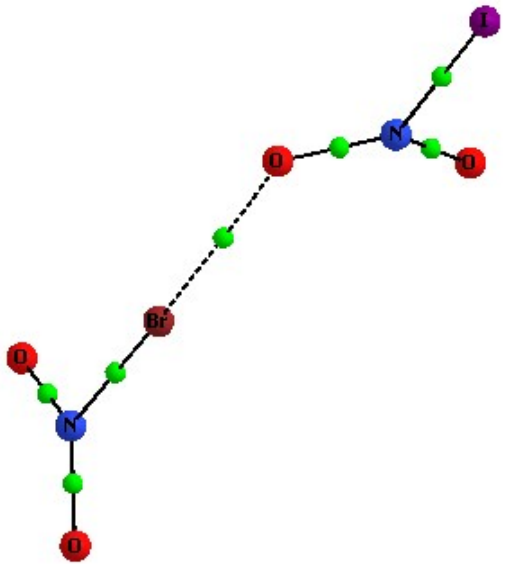
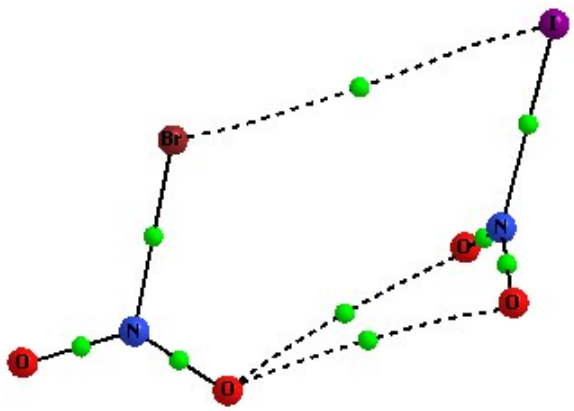
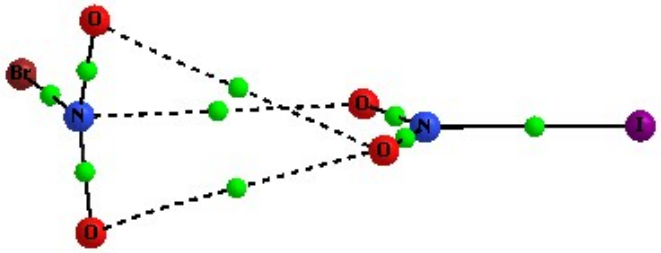
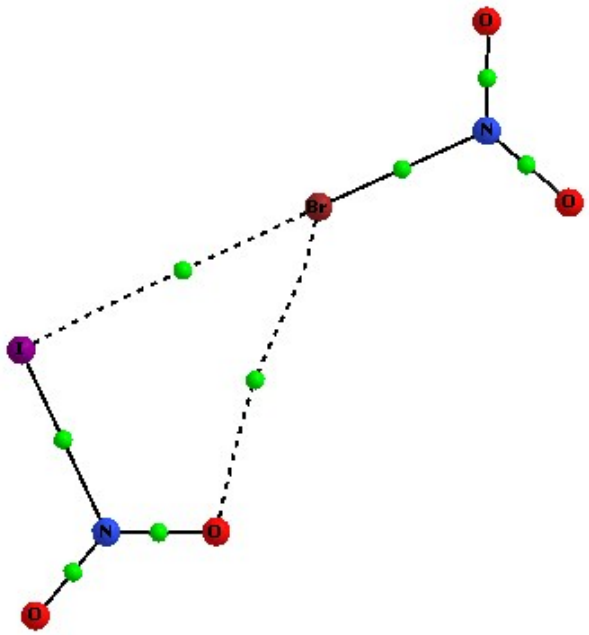
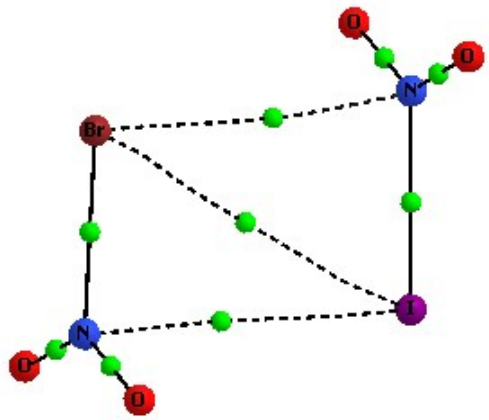
	
BrI_{4a} 	N 0.166905 -4.463256 0.000000 O 0.240410 -4.958904 1.092796 O 0.240410 -4.958904 -1.092796 N 0.240410 1.218969 0.000000 O 1.403594 0.893893 0.000000 O -0.747095 0.518367 0.000000 I -0.142174 3.351577 0.000000 Br -0.126129 -2.482263 0.000000
BrI_{5a} 	N -2.652686 -1.455730 0.000000 O -2.834670 -0.272205 0.000000 O -3.404289 -2.386429 0.000000 N -0.180500 1.612613 0.000000 O -0.678856 1.719397 1.092092 O -0.678856 1.719397 -1.092092 I 1.969163 1.168269 0.000000 Br -0.678856 -1.978792 0.000000
BrI_{6a}	N 1.153455 -2.404381 0.000000 O 1.560827 -2.135596 1.093284 O 1.560827 -2.135596 -1.093284 N 0.355386 0.991014 0.000000 O 1.560827 0.925409 0.000000

	O -0.458420 0.097509 0.000000 I -0.478271 3.003513 0.000000 Br -0.543030 -3.523042 0.000000
BrI_{1b} 	N 1.173609 -2.383864 0.000000 O 1.358628 -3.573600 0.000000 O 1.958173 -1.471553 0.000000 N 0.574750 3.651296 0.000000 O -0.332327 4.437625 0.000000 O 1.763954 3.815038 0.000000 Br 0.000000 1.711467 0.000000 I -0.947659 -1.781763 0.000000
BrI_{2b} 	N 0.050542 -2.017263 0.000000 O -0.344107 -2.340971 1.092286 O -0.344107 -2.340971 -1.092286 N -0.703648 2.204360 0.000000 O -0.344107 2.535433 1.093792 O -0.344107 2.535433 -1.093792 I 1.741851 -0.632030 0.000000 Br -2.192426 0.830759 0.000000
BrI_{3b}	N -1.565269 1.077726 0.209966 O -1.038514 1.549496 -0.759971 O -1.504022 1.371694 1.369552 N 1.906823 1.222504 -0.181907 O 2.228667 1.544808 -1.296301 O 1.733568 1.894145 0.803536

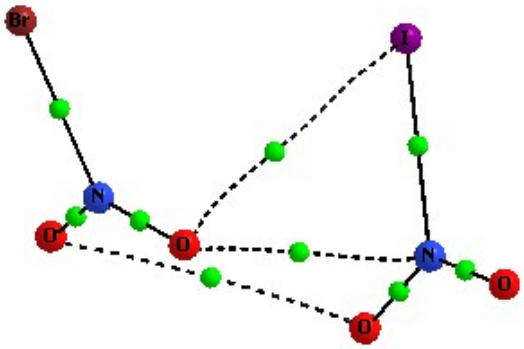
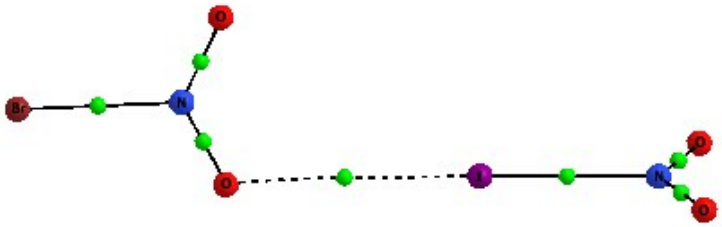
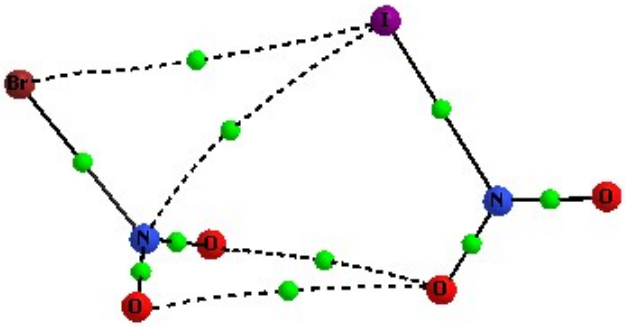
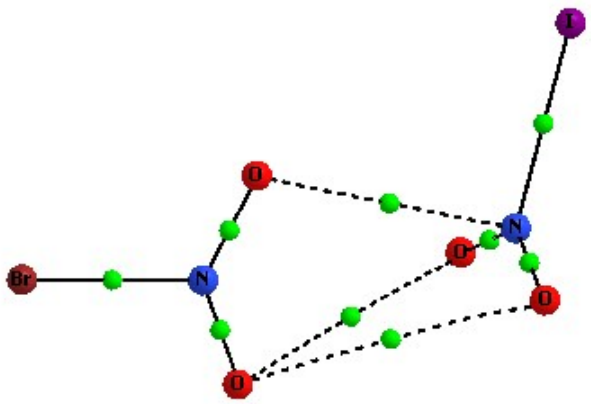
	I 1.568707 -0.932611 0.103241 Br -2.768284 -0.501553 -0.188648
BrI_{4b} 	N 0.176773 -3.775749 0.000000 O 0.255154 -4.293166 1.091346 O 0.255154 -4.293166 -1.091346 N 0.255154 2.091990 0.000000 O 1.421049 1.804967 0.000000 O -0.724837 1.389219 0.000000 I -0.148296 -1.634716 0.000000 Br -0.137599 4.044669 0.000000
BrI_{5b} 	N 0.800931 2.409105 0.000000 O 1.792943 1.722072 0.000000 O 0.689459 3.608618 0.000000 N 1.412994 -1.517714 0.000000 O 1.792943 -1.218640 1.094055 O 1.792943 -1.218640 -1.094055 I -1.084483 1.289664 0.000000 Br -0.187605 -2.792548 0.000000
BrI_{6b} 	N 1.882548 0.208106 0.000000 O 1.882548 0.721110 1.091575 O 1.882548 0.721110 -1.091575 N -1.394561 1.384071 0.000000 O -0.704557 2.363817 0.000000 O -1.115138 0.216846 0.000000 I 1.876163 -1.977137 0.000000 Br -3.383307 1.756000 0.000000

Table S2. Interatomic interaction distances (Å) for all the complexes studied.

FCl	X-Y	X-N	Y-N	O-O	X-O	Y-O	N-O
1a	3.0468	-	-	-	-	-	-
2a	-	2.8652	3.3231	3.3237	-	-	-
3a	-	-	-	3.1226	3.2567	-	-
4a	-	-	-	-	-	-	-
5a	-		-		-	-	-
6a	-	-	-	3.2395	-	-	2.9760
1b	-	-	-	-	-	-	-
2b	-	2.8666	3.3192	-	-	-	-
3b	-	-	-	3.2281	-	3.3672	-
4b	-	-	-	-	-	3.2088	-
5b	-	-	3.4082	3.0901	-	-	-
6b	-	-	-	3.3694	-	-	2.9650
FBr	**X-Y**	**X-N**	**Y-N**	**O-O**	**X-O**	**Y-O**	**N-O**
1a	3.05194	-	-	-	-	-	-
2a	-	2.8946	-	3.2454	-	-	-
3a	-	2.9895	-	3.2504	-	-	-
4a	-	-	-	-	-	-	-
5a	3.5652	-	-	3.1327	-	-	-
6a	-	-	-	3.2600	-	2.9546	-
1b	-	-	-	-	-	-	-
2b	-	-	3.4982	-	-	-	-
3b	-	-	-	3.3056	-	3.5855	-
4b	-	-	-	-	-	3.2515	-
5b	3.6335	-	3.5528	3.0853	-	-	-
6b	-	-	-	3.2225	-	3.0248	-
FI	**X-Y**	**X-N**	**Y-N**	**O-O**	**X-O**	**Y-O**	**N-O**
1a	2.9990	-	-	-	-	-	-
2a	3.5916	-	-	3.2852	-	-	-
3a	-	2.9173	-	3.1923	-	-	-
4a	-	-	-	-	-	-	-
5a	3.6271	-	-	3.0664	-	-	-
6a	-	-	-	3.1807	-	-	2.9610
1b	-	-	-	-	-	-	-
2b	3.6300	2.9406	-	-	-	-	-
3b	-	-	3.6854	3.3068	-	-	-
4b	-	-	-	-	-	3.2060	-
5b	3.7540	-	-	3.1141	-	-	-
6b	-	-	-	3.2462	-	3.0066	-
ClBr	**X-Y**	**X-N**	**Y-N**	**O-O**	**X-O**	**Y-O**	**N-O**
1a	3.4715	-	-	-	-	-	-
2a	3.8888	3.4196	3.5659	3.1830	-	-	-
3a	-	-	-	-	3.4030	-	2.9769
4a	-	-	-	-	3.1141	-	-
5a	3.8663	3.4369	-	3.1452	-	-	-

6a	-	-	-	3.2860	-	-	2.9647
1b	3.5753	-	-	-	3.6253	-	-
2b	3.9583	3.4247	3.5633	-	-	-	-
3b	-	-	-	-	-	3.5422	3.0077
4b	-	-	-	-	-	3.1490	-
5b	3.9141	-	3.5884	3.1368	-	-	-
6b	-	-	-	3.2856	-	-	2.9856
ClI	**X-Y**	**X-N**	**Y-N**	**O-O**	**X-O**	**Y-O**	**N-O**
1a	3.3959					3.7317	
2a	4.0133	3.4602	3.7131	3.2034	-	-	-
3a	-	-	-	3.3123	3.4118	-	2.9448
4a	-	-	-	-	3.0694	-	-
5a	3.9395	-	-	3.1429	-	-	-
6a	-	-	-	3.2651	-	-	2.9547
1b	3.64026	-	-	-	3.6683	-	-
2b	4.0662	3.4619	3.7222	-	-	-	-
3b	-	-	-	3.2045	-	3.6953	3.0370
4b	-	-	-	-	-	3.1076	-
5b	4.0611	-	-	3.1364	-	-	-
6b	-	-	-	3.2883	-	-	2.9904
BrI	**X-Y**	**X-N**	**Y-N**	**O-O**	**X-O**	**Y-O**	**N-O**
1a	3.4807	-	-	-	-	3.7606	-
2a	4.1532	3.6213	3.7335	3.1965	-	-	-
3a	-	-	-	3.3015	-	-	2.9601
4a	-	-	-	-	3.0642	-	-
5a	4.1129	-	-	3.1316	-	-	-
6a	-	-	-	3.2504	-	-	2.9762
1b	3.6195	-	-	-	3.7371	-	-
2b	4.1974	3.6252	3.7451	-	-	-	-
3b	-	-	-	3.3280	-	3.7018	3.0193
4b	-	-	-	-	-	3.0784	-
5b	4.1796	-	3.7575	3.1376	-	-	-
6b	-	-	-	3.2532	-	-	2.9977

Table S3. Electron density (ρ_{BCP}) and Laplacian ($\nabla^2\rho_{BCP}$) in a.u. at MP2/aug-cc-pVTZ computational level.

	X···Y		X···N		Y···N		O···O		X···O		Y···O		N···O	
XY	**ρ**	**$\nabla^2\rho$**	**ρ**	**$\nabla^2\rho$**	**ρ**	**$\nabla^2\rho$**	**ρ**	**$\nabla^2\rho$**	**ρ**	**$\nabla^2\rho$**	**ρ**	**$\nabla^2\rho$**	**ρ**	**$\nabla^2\rho$**
FCl														
1a	0.0063	0.0315	-	-	-	-	-	-	-	-	-	-	-	-
2a	-	-	0.0065	0.0368	0.0051	0.0255	0.0033	0.0137	-	-	-	-	-	-
3a	-	-	-	-	-	-	0.0039	0.0170	0.0046	0.0221	-	-	-	-
4a	-	-	-	-	-	-	-	-	-	-	-	-	-	-
5a	-	-	0.0068	0.0388	-	-	0.0050	0.0232	-	-	-	-	-	-
6a	-	-	-	-	-	-	0.0041	0.0176	-	-	-	-	0.0061	0.0325
1b	-	-	-	-	-	-	-	-	-	-	-	-	-	-
2b	-	-	0.0064	0.0363	0.0052	0.0256	-	-	-	-	-	-	-	-
3b	-	-	-	-	-	-	0.0043	0.0183	-	-	0.0061	0.0278	-	-
4b	-	-	-	-	-	-	-	-	-	-	0.0055	0.0250	-	-
5b	-	-	-	-	0.0041	0.0209	0.0053	0.0251	-	-	-	-	-	-
6b	-	-	-	-	-	-	0.0030	0.0136	-	-	-	-	0.0064	0.0341
FBr														
1a	0.0093	0.0367	-	-	-	-	-	-	-	-	-	-	-	-
2a	-	-	0.0073	0.0351	-	-	0.0039	0.0151	-	-	-	-	-	-
3a	-	-	0.0062	0.0304	-	-	0.0041	0.0174	-	-	-	-	-	-
4a	-	-	-	-	-	-	-	-	-	-	-	-	-	-
5a	0.0042	0.0156	-	-	-	-	0.0051	0.0218	-	-	-	-	-	-
6a	-	-	-	-	-	-	0.0044	0.0172	-	-	-	-	0.0071	0.0334
1b	-	-	-	-	-	-	-	-	-	-	-	-	-	-
2b	-	-	-	-	0.0051	0.0213	-	-	-	-	-	-	-	-
3b	-	-	-	-	-	-	0.0038	0.0148	-	-	0.0051	0.0189	-	-
4b	-	-	-	-	-	-	-	-	-	-	0.0072	0.0264	-	-
5b	0.0043	0.0165	-	-	0.0045	0.0193	0.0057	0.0246	-	-	-	-	-	-
6b	-	-	-	-	-	-	0.0046	0.0176	-	-	-	-	0.0063	0.0296
FI														
1a	0.0130	0.0485	-	-	-	-	-	-	-	-	-	-	-	-
2a	0.0063	0.0196	-	-	-	-	0.0036	0.0134	-	-	-	-	-	-
3a	-	-	0.0073	0.0355	-	-	0.0046	0.0197	-	-	-	-	-	-
4a														
5a	0.0050	0.0164	-	-	-	-	0.0058	0.0259	-	-	-	-	-	
6a	-	-	-	-	-	-	0.0052	0.0199	-	-	-	-	0.0073	0.0339
1b	-	-	-	-	-	-	-	-	-	-	-	-	-	-
2b	0.0060	0.0194	0.0065	0.0309	-	-	-	-	-	-	-	-	-	-
3b	-	-	-	-	0.0052	0.0197	0.0038	0.0145	-	-	-	-	-	-
4b	-	-	-	-	-	-	-	-	-	-	0.0099	0.0345	-	-
5b	0.0047	0.0151	-	-	-	-	0.0054	0.0230	-	-	-	-	-	-
6b	-	-	-	-	-	-	0.0043	0.0168	-	-	-	-	0.0067	0.0307
ClBr														
1a	0.0083	0.0280	-	-	-	-	-	-	-	-	-	-	-	-

2a	0.0052	0.0167	0.0051	0.0210	0.0048	0.0188	0.0044	0.0168	-	-	-	-	-	-
3a	-	-	-	-	-	-	-	-	0.0061	0.0234	-	-	0.0065	0.0308
4a	-	-	-	-	-	-	-	-	0.0078	0.0313	-	-	-	-
5a	0.0050	0.0162	0.0049	0.0202	-	-	0.0050	0.0203	-	-	-	-	-	-
6a	-	-	-	-	-	-	0.0041	0.0159	-	-	-	-	0.0072	0.0332
1b	0.0069	0.0238	-	-	-	-	-	-	0.0033	0.0117	-	-	-	-
2b	0.0046	0.0149	0.0050	0.0206	0.0048	0.0188	-	-	-	-	-	-	-	-
3b	-	-	-	-	-	-	-	-	-	-	0.0058	0.0206	0.0062	0.0287
4b	-	-	-	-	-	-	-	-	-	-	0.0089	0.0327	-	-
5b	0.0047	0.0151	-	-	0.0046	0.0178	0.0051	0.0207	-	-	-	-	-	-
6b	-	-	-	-	-	-	0.0041	0.0157	-	-	-	-	0.0069	0.0319
ClI														
1a	0.0106	0.0363	-	-	-	-	-	-	-	-	0.0041	0.0141	-	-
2a	0.0047	0.0251	0.0043	0.0191	0.0044	0.0175	0.0042	0.0171	-	-	-	-	-	-
3a	-	-	-	-	-	-	0.0035	0.0140	0.0059	0.0227	-	-	0.0068	0.0327
4a	-	-	-	-	-	-	-	-	0.0075	0.0345	-	-	-	-
5a	0.0051	0.0162	-	-	-	-	0.0047	0.0210	-	-	-	-	-	-
6a	-	-	-	-	-	-	0.0039	0.0166	-	-	-	-	0.0067	0.0345
1b	0.0076	0.0251	-	-	-	-	-	-	0.0029	0.0112	-	-	-	-
2b	0.0043	0.0138	0.0043	0.0190	0.0044	0.0176	-	-	-	-	-	-	-	-
3b	-	-	-	-	-	-	0.0032	0.0134	-	-	0.0053	0.0178	0.0056	0.0271
4b	-	-	-	-	-	-	-	-	-	-	0.0075	0.0345	-	-
5b	0.0046	0.0143	-	-	-	-	0.0049	0.0215	-	-	-	-	-	-
6b	-	-	-	-	-	-	0.0037	0.0155	-	-	-	-	0.0063	0.0321
BrI														
1a	0.0115	0.0344	-	-	-	-	-	-	-	-	0.0404	0.0137	-	-
2a	0.0045	0.0138	0.0040	0.0166	0.0043	0.0168	0.0043	0.0173	-	-	-	-	-	-
3a	-	-	-	-	-	-	0.0036	0.0140	-	-	-	-	0.0067	0.0316
4a	-	-	-	-	-	-	-	-	0.00925	0.0388	-	-	-	-
5a	0.0048	0.0142	-	-	-	-	0.0048	0.0214	-	-	-	-	-	
6a	-	-	-	-	-	-	0.0040	0.0170	-	-	-	-	0.0065	0.0329
1b	0.0096	0.0278	-	-	-	-	-	-	0.0032	0.0121	-	-	-	-
2b	0.0042	0.0128	0.0040	0.0167	0.0043	0.0169	-	-	-	-	-	-	-	-
3b	-	-	-	-	-	-	0.0034	0.0140	-	-	0.0052	0.0176	0.0058	0.0283
4b	-	-	-	-	-	-	-	-	-	-	0.0111	0.0436	-	-
5b	0.0046	0.0135	-	-	0.0041	0.0158	0.0048	0.0213	-	-	-	-	-	-
6b	-	-	-	-	-	-	0.0040	0.0168	-	-	-	-	0.0063	0.0315

Table S4. Total Electron density energy (H_{BCP}) in a.u at MP2/aug-cc-pVTZ computational level.

	X···Y	X···N	Y···N	O···O	X···O	Y···O	N···O
FCl	**H**	**H**	**H**	in a.u	**H**	**H**	**H**
1a	0.0017						
2a		0.0020	0.0016	0.0007			
3a				0.0009	0.0010		
4a							
5a		0.0022		0.0012			
6a				0.0009			0.0019
1b							
2b		0.0020	0.0016				
3b				0.0010		0.0016	
4b						0.0014	
5b			0.0014	0.0014			
6b				0.0007			0.0020
FBr							
1a	0.0014						
2a		0.0017		0.0007			
3a		0.0014		0.0009			
4a							
5a	0.0007			0.0011			
6a				0.0008		0.0018	
1b							
2b			0.0013				
3b				0.0007		0.0009	
4b						0.0012	
5b	0.0008		0.0012	0.0013			
6b				0.0008			0.0016
FI							
1a	0.0014						
2a	0.0006			0.0006			
3a		0.0016		0.0010			
4a							
5a	0.0006			0.0014			
6a				0.0009			0.0017
1b							
2b	0.0006	0.0016					
3b			0.0010	0.0007			
4b						0.0013	
5b	0.0006			0.0011			
6b				0.0007		0.0000	0.0017
ClBr							
1a	0.0013						
2a	0.0008	0.0012	0.0011	0.0008			
3a					0.0011		0.0017

4a					0.0016		
5a	0.0009	0.0012		0.0010			
6a				0.0007			0.0018
1b	0.0012				0.0006		
2b	0.0008	0.0012	0.0011				
3b						0.0010	0.0016
4b						0.0014	
5b	0.0008		0.0010	0.0010			
6b				0.0007			0.0017
ClI							
1a	0.0014					0.0007	
2a	0.0008	0.0012	0.0010	0.0008			
3a				0.0007	0.0012		0.0019
4a					0.0019		
5a	0.0009			0.0011			
6a				0.0008			0.0020
1b	0.0012				0.0006		
2b	0.0007	0.0012	0.0010				
3b				0.0006		0.0008	0.0016
4b						0.0017	
5b	0.0008			0.0011			
6b				0.0008			0.0019
BrI							
1a	0.0009					0.0007	
2a	0.0007	0.0010	0.0010	0.0008			
3a				0.0007			0.0019
4a					0.0018		
5a	0.0007			0.0011			
6a				0.0008			0.0019
1b	0.0009				0.0007		
2b	0.0007	0.0011	0.0010				
3b				0.0007		0.0008	0.0016
4b						0.0017	
5b	0.0007		0.0010	0.0011			
6b				0.0008			0.0018

Table S5. Total NBO charge (in a.u.) of monomer NO_2X in the complexes at MP2/aug-cc-pVTZ computational level.

	Comp.	Charge	Comp.	Charge		Comp.	Charge	Comp.	Charge
FCl	1a	0.0049	1b	-	**ClBr**	1a	0.0140	1b	-0.0138
	2a	-0.0004	2b	-0.0004		2a	-0.0003	2b	-0.0003
	3a	-0.0021	3b	0.0003		3a	-0.0025	3b	0.0016
	4a	-	4b	0.0050		4a	-0.0103	4b	0.0102
	5a	-0.0015	5b	-0.0002		5a	-0.0021	5b	0.0008
	6a	-0.0028	6b	-0.0006		6a	-0.0023	6b	0.0012
FBr	1a	0.0057	1b	-	**ClI**	1a	0.0254	1b	-0.0254
	2a	-0.0006	2b	-0.0002		2a	-0.0004	2b	-0.0002
	3a	-0.0023	3b	0.0001		3a	-0.0031	3b	0.0011
	4a	-	4b	0.0053		4a	-0.0136	4b	0.0171
	5a	-0.0018	5b	-0.0006		5a	-0.0035	5b	0.0002
	6a	-0.0037	6b	-0.0010		6a	-0.0035	6b	0.0002
FI	1a	0.0103	1b	-	**BrI**	1a	0.0378	1b	-0.0401
	2a	-0.0011	2b	-0.0009		2a	0.0000	2b	0.0003
	3a	-0.0032	3b	-0.0003		3a	-0.0027	3b	0.0015
	4a	-	4b	0.0095		4a	-0.0171	4b	0.0202
	5a	-0.0031	5b	-0.0012		5a	-0.0027	5b	0.0007
	6a	-0.0046	6b	-0.0017		6a	-0.0031	6b	0.0008