Supplementary Information for:

Intermolecular Interactions in Clusters of Ethylammonium Nitrate and 1-Amino-1,2,3-triazole

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1. List of unique QUAOs for the $(EAN)_n$ (n=1-8)

Table S1.1. Atoms participating in bonding interactions (Atom1 and Atom2), bond orders (BOs) and KBOs (kcal/mol) for H-bonds in $(EAN)_n$ (n= 1-6) IL clusters. Atom numbers in Atom1 and Atom2 are labeled in Figure 2a through Figure 2e. *R* represents the H-bond distance in Å. Occ(Atom1) and Occ(Atom2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively. Orbital (Atom1) and Orbital (Atom2) are types of orbitals in Atom1 and Atom2 participating in the H-bonding interactions, respectively. The KBOs in parentheses is the sum of the H-bond and N···O KBOs.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R (Å)	Occ (Atom1)	Orbital (Atom 1)	Occ (Atom2)	Orbital (Atom2)
$(EAN)_1$	O12	H5	0.33	-5.66 (-6.65)	1.75	1.91	*p*l *(horizontal)*	0.61	*σ*
	O12	H5	0.10	-0.69 (-0.86)	1.75	1.82	*p*l *(perpendicular)*	0.61	*σ*
$(EAN)_2$	O12	H5	0.30	-5.14 (-6.87)	1.75	1.92	*p*l	0.63	*σ*
	O27	H20	0.29	-4.90 (-6.47)	1.75	1.92	*pl*	0.61	*σ*
	O27	H6	0.22	-2.78 (-3.80)	1.83	1.95	*pl*	0.64	*σ*
	O15	H20	0.10	-0.80 (-1.06)	2.03	1.98	*sl*	0.61	*σ*
$(EAN)_4$	O42	H35	0.30	-5.23 (-6.97)	1.75	1.92	*pl*	0.63	*σ*
	O57	H50	0.30	-4.99 (-6.64)	1.75	1.92	*pl*	0.63	*σ*
	O27	H20	0.29	-4.93 (-6.59)	1.75	1.92	*pl*	0.63	*σ*
	H21	O12	0.28	-4.60 (-6.27)	1.75	0.63	*pl*	1.92	*σ*
	O12	H5	0.28	-4.69 (-6.30)	1.75	1.93	*pl*	0.63	*σ*
	H21	O12	0.23	-2.87 (-3.88)	1.80	0.64	*σ*	0.64	*pl*
	O59	H36	0.12	-2.32 (-3.21)	1.90	0.67	*σ*	0.65	*pl*
$(EAN)_6$	O72	H65	0.30	-5.09 (-6.80)	1.75	1.91	*pl*	0.63	*σ*
	O87	H80	0.29	-4.98 (-6.65)	1.75	1.92	*pl*	0.63	*σ*
	O42	H35	0.29	-4.97 (-6.65)	1.75	1.92	*pl*	0.61	*σ*
	O12	H5	0.28	-4.72 (-6.27)	1.75	1.93	*pl*	0.62	*σ*
	O27	H20	0.27	-4.46 (-5.91)	1.75	1.93	*pl*	0.63	*σ*
	O57	H50	0.28	-4.49 (-5.98)	1.75	1.93	*pl*	0.63	*σ*
	H81	O57	0.22	-2.83 (-4.49)	1.78	0.64	*σ*	1.94	*pl*
	H51	O29	0.20	-2.83 (-3.84)	1.86	0.64	*σ*	1.94	*pl*
	H7	O44	0.16	-1.48 (-2.04)	1.98	0.65	*σ*	1.96	*pl*

Table S1.2. Atoms participating in bonding interactions, bond orders (BOs) and KBOs (kcal/mol) for H-bonds in $(EAN)_8$ IL clusters. Atom numbers in Atom1 and Atom2 are labeled in Figure 2e. *R* represents the H-bond distance in Å. Occ(Atom1) and Occ(Atom2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively. Orbital (Atom1) and Orbital (Atom2) are types of orbitals in Atom1 and Atom2 participating in the H-bonding interactions, respectively. The KBOs in parentheses is the sum of the H-bond and N···O KBOs.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R (Å)	Occ (Atom1)	Orbital (Atom 1)	Occ (Atom2)	Orbital (Atom2)
$(EAN)_8$	O117	H110	0.30	-5.09 (-6.79)	1.75	1.92	*pl*	0.63	*σ*
	O102	H95	0.30	-5.06 (-6.76)	1.75	1.92	*pl*	0.63	*σ*
	O42	H35	0.28	-4.82 (-6.41)	1.75	1.92	*pl*	0.61	*σ*
	O12	H5	0.28	-4.68 (-6.20)	1.75	1.92	*pl*	0.62	*σ*
	O87	H80	0.27	-4.68 (-6.20)	1.75	1.93	*pl*	0.62	*σ*
	O27	H20	0.27	-4.60 (-6.20)	1.75	1.93	*pl*	0.63	*σ*
	O57	H50	0.27	-4.58 (-6.08)	1.75	1.93	*pl*	0.62	*σ*
	O72	H65	0.27	-4.53 (-6.04)	1.75	1.93	*pl*	0.63	*σ*
	H96	O72	0.23	-3.11 (-4.22)	1.81	0.64	*σ*	1.94	*pl*
	H21	O12	0.22	-2.90 (-3.95)	1.80	0.65	*σ*	1.94	*pl*
	H51	O42	0.19	-2.13 (-3.00)	1.95	0.67	*σ*	1.96	*pl*
	H111	O87	0.18	-2.03 (-2.86)	1.96	0.66	*σ*	1.96	*pl*
	H66	O27	0.18	-1.99 (-2.76)	1.89	0.65	*σ*	1.96	*pl*
	H52	O29	0.18	-2.04 (-2.75)	1.93	0.67	*σ*	1.90	*pl*
	H112	O104	0.15	-1.49 (-1.95)	1.96	0.67	*σ*	1.90	*pl*
	H112	O104	0.12	-0.91 (-1.35)	1.96	0.67	*σ*	1.98	*sl*

2. List of unique QUAOs for the $(EAN)_{10}$ to $(EAN)_{16}$

Table S2.1. Atoms participating in bonding interactions (Atom1 and Atom2), bond orders (BOs) and KBOs (kcal/mol) for H-bonds in $(EAN)_{10}$ IL clusters. Atom numbers in Atom1 and Atom2 are labeled in Figure 2f. *R* represents the H-bond distance in Å. Occ(Atom1) and Occ(Atom2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively. Orbital (Atom1) and Orbital (Atom2) are types of orbitals in Atom1 and Atom2 participating in the H-bonding interactions, respectively. The KBOs in parentheses is the sum of the H-bond and N···O KBOs.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R (Å)	Occ (Atom1)	Orbital (Atom 1)	Occ (Atom2)	Orbital (Atom2)
$(EAN)_{10}$	O132	H125	0.32	-5.44 (-7.20)	1.75	1.91	*p*l	0.61	*σ*
	O147	H140	0.31	-5.31 (-7.07)	1.75	1.82	*p*l	0.61	*σ*
	O42	H35	0.29	-5.05 (-6.66)	1.75	1.91	*p*l	0.61	*σ*
	O12	H5	0.29	-4.94 (-6.53)	1.75	1.91	*p*l	0.62	*σ*
	O87	H80	0.28	-4.74 (-6.28)	1.75	1.92	*p*l	0.61	*σ*
	O72	H65	0.28	-4.24 (-6.26)	1.75	1.92	*p*l	0.61	*σ*
	O102	H95	0.28	-4.61 (-6.10)	1.75	1.93	*p*l	0.62	*σ*
	O57	H50	0.27	-4.60 (-6.10)	1.75	1.93	*p*l	0.62	*σ*
	O27	H20	0.27	-4.58 (-6.06)	1.75	1.93	*p*l	0.62	*σ*
	O117	H110	0.27	-4.55 (-6.05)	1.75	1.93	*p*l	0.62	*σ*
	H111	O117	0.27	-4.09 (-5.58)	1.75	1.93	*σ*	0.62	*p*l
	H111	O115	0.25	-3.61 (-4.97)	1.75	1.93	*σ*	0.63	*p*l
	H52	O30	0.23	-3.19 (-4.34)	1.88	0.63	*σ*	1.93	*p*l
	H21	O12	0.22	-2.83 (-3.84)	1.82	0.65	*σ*	1.94	*p*l
	H96	O72	0.20	2.42 (-3.33)	1.89	0.66	*σ*	1.91	*p*l
	H81	O57	0.19	-2.12 (-2.91)	1.95	0.64	*σ*	1.95	*p*l
	H66	O27	0.19	-2.09 (-2.88)	1.96	0.64	*σ*	1.95	*p*l
	H51	O42	0.22	-2.86 (-3.95)	1.85	0.64	*σ*	1.95	*p*l

Table S2.2. Atoms participating in bonding interactions (Atom1 and Atom2), bond orders (BOs) and KBOs (kcal/mol) for H-bonds in $(EAN)_{12}$ IL clusters. Atom numbers in Atom1 and Atom2 are labeled in Figure 2g. *R* represents the H-bond distance in Å. Occ(Atom1) and Occ(Atom2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively. Orbital (Atom1) and Orbital (Atom2) are types of orbitals in Atom1 and Atom2 participating in the H-bonding interactions, respectively. The KBOs in parentheses is the sum of the H-bond and N···O KBOs.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R (Å)	Occ (Atom1)	Orbital (Atom 1)	Occ (Atom2)	Orbital (Atom2)
$(EAN)_{12}$	O177	H170	0.32	-5.44 (-7.33)	1.75	1.91	*p*l	0.61	*σ*
	O132	H125	0.31	-5.31 (-6.96)	1.75	1.91	*p*l	0.62	*σ*
	O147	H140	0.30	-5.05 (-6.88)	1.75	1.92	*p*l	0.61	*σ*
	O42	H35	0.30	-4.94 (-6.77)	1.75	1.92	*p*l	0.61	*σ*
	O162	H155	0.30	-4.74 (-6.69)	1.75	1.93	*p*l	0.62	*σ*
	O102	H95	0.28	-4.72 (-6.30)	1.75	1.93	*p*l	0.62	*σ*
	O72	H65	0.28	-4.61 (-6.15)	1.75	1.93	*p*l	0.62	*σ*
	O87	H80	0.28	-4.60 (-6.20)	1.75	1.93	*p*l	0.62	*σ*
	O27	H20	0.28	-4.58 (-6.08)	1.75	1.93	*p*l	0.62	*σ*
	O117	H110	0.28	-4.55 (-6.19)	1.75	1.93	*p*l	0.63	*σ*
	O57	H50	0.28	-4.09 (-6.12)	1.75	0.63	*σ*	1.93	*p*l
	H156	O14	0.24	-3.61 (-4.58)	1.87	0.65	*σ*	1.94	*p*l
	H141	O117	0.24	-3.19 (-4.25)	1.81	0.66	*σ*	1.91	*p*l
	H111	O72	0.22	-2.83 (-3.86)	2.04	0.64	*σ*	1.95	*p*l
	H 81	O57	0.21	-2.42 (-3.73)	2.04	0.64	*σ*	1.95	*p*l
	H126	O150	0.21	-2.30 (-3.95)	1.95	0.65	*σ*	1.92	*p*l
	H142	O104	0.21	-2.44 (-2.88)	1.95	0.65	*σ*	1.91	*p*l
	H51	O57	0.21	-2.08 (-2.37)	1.99	0.68	*σ*	1.96	*p*l
	H50	O90	0.20	-2.02 (-2.33)	2.03	0.65	*σ*	1.95	*p*l

Table S2.3. Atoms participating in bonding interactions (Atom1 and Atom2), Bond orders (BOs) and KBOs (kcal/mol) for H-bonds in $(EAN)_{16}$ IL clusters. Atom numbers in Atom1 and Atom2 are labeled in Figure 2h. *R* represents the H-bond distance in Å. Occ(Atom1) and Occ(Atom2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively. Orbital (Atom1) and Orbital (Atom2) are types of orbitals in Atom1 and Atom2 participating in the H-bonding interactions, respectively. The KBOs in parentheses is the sum of the H-bond and N···O KBOs.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R (Å)	Occ (Atom1)	Orbital (Atom 1)	Occ (Atom2)	Orbital (Atom2)
$(EAN)_{16}$	O112	H110	0.31	-5.25 (-6.99)	1.75	1.91	*p*l	0.62	*σ*
	O102	H95	0.30	-5.19 (-6.91)	1.75	1.91	*p*l	0.63	*σ*
	O237	H230	0.30	-5.03 (-6.71)	1.75	1.92	*p*l	0.63	*σ*
	O147	H140	0.30	-4.96 (-6.55)	1.75	1.92	*p*l	0.62	*σ*
	O222	H215	0.29	-4.96 (-6.56)	1.75	1.92	*p*l	0.62	*σ*
	O132	H125	0.29	-4.93 (-6.50)	1.75	1.92	*p*l	0.61	*σ*
	O12	H5	0.29	-4.86 (-6.44)	1.75	1.92	*p*l	0.62	*σ*
	O177	H170	0.28	-4.77 (-6.30)	1.75	1.92	*p*l	0.62	*σ*
	O192	H185	0.28	-4.66 (-6.17)	1.75	1.92	*p*l	0.63	*σ*
	O 87	H80	0.28	-4.76 (-4.65)	1.75	1.93	*p*l	0.62	*σ*
	O 57	H50	0.28	-4.67 (-6.18)	1.75	1.93	*p*l	0.62	*σ*
	O 42	H35	0.28	-4.61 (-4.65)	1.75	1.92	*p*l	0.64	*σ*
	O 27	H20	0.28	-4.67 (-6.18)	1.75	1.93	*p*l	0.63	*σ*
	O 72	H65	0.27	-4.58 (-6.09)	1.75	1.93	*p*l	0.63	*σ*
	O207	H200	0.27	-4.55 (-6.06)	1.75	1.93	*p*l	0.62	*σ*
	O162	H155	0.27	-4.55 (-6.06)	1.75	1.93	*p*l	0.63	*σ*
	H231	O207	0.27	-4.22 (-5.69)	1.75	0.63	*σ*	1.93	*p*l
	H 96	O74	0.24	-3.21 (-4.34)	1.77	0.63	*σ*	1.94	*p*l
	H186	O162	0.22	-2.98 (-4.13)	1.85	0.64	*σ*	1.95	*p*l
	H 81	O57	0.22	-2.71 (-3.68)	1.86	0.65	*σ*	1.95	*p*l
	H66	O27	0.18	-1.99 (-2.75)	1.89	0.64	*σ*	1.96	*p*l
	H171	O147	0.22	-2.82 (-3.93)	1.89	0.64	*σ*	1.96	*p*l
	H201	O177	0.14	-1.16 (-1.49)	1.89	0.66	*σ*	1.81	*p*l
	H112	O102	0.16	-1.40 (-1.98)	1.92	0.65	*σ*	1.96	*p*l
	H7	O44	0.13	-1.16 (-1.63)	2.02	0.67	*σ*	1.98	*p*l
	H 21	O14	0.13	-1.01 (-1.37)	2.04	0.66	*σ*	1.94	*p*l
	H185	O225	0.11	-1.06 (-1.53)	2.04	0.65	*σ*	1.96	*sl*
	H187	O59	0.12	-1.09 (-1.55)	2.04	0.67	*σ*	1.98	*p*l

3. List of unique QUAOs for the $N\cdots O$ interactions

Table S3.1. Atoms participating in bonding interactions (Atom1 and Atom2), bond orders (BO), KBOs (kcal/mol) of the $N\cdots O$ interactions in $(EAN)_n$ (n=1-8). Atom numbers in Atom1 and Atom2 are labeled in Figure 2a through Figure 2e. The $N\cdots O$ distances (R) are in Å. Occ(Atom1) and Occ(Atom2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R(Å)	Occ (Atom1)	Occ (Atom2)
$(EAN)_1$	O12	N4	0.20	-1.86	2.58	1.91	1.46
	O12	N4	0.06	-0.17	2.58	1.82	1.46
$(EAN)_2$	O12	N4	0.19	-1.72	2.70	1.92	1.44
	O27	N19	0.18	-1.57	2.70	1.92	1.46
	O27	N4	0.15	-1.02	2.69	1.95	1.41
	O15	N19	0.07	-0.26	2.63	1.98	1.46
$(EAN)_4$	O42	N34	0.19	-1.73	2.70	1.91	1.44
	O57	N49	0.19	-1.65	2.70	1.92	1.43
	O27	N19	0.18	-1.66	2.70	1.92	1.45
	N19	O12	0.17	-1.67	2.65	1.44	1.94
	O12	N4	0.18	-1.61	2.71	1.93	1.42
	N49	O30	0.15	-1.01	2.79	1.39	1.90
	O44	N4	0.09	-0.86	2.79	1.37	1.37
$(EAN)_6$	O72	N64	0.19	-1.71	2.70	1.91	1.44
	O87	N79	0.19	-1.67	2.70	1.92	1.43
	O42	N34	0.18	-1.61	2.70	1.92	1.45
	O12	N4	0.18	-1.54	2.70	1.93	1.44
	O27	N19	0.17	-1.45	2.69	1.93	1.43
	O57	N49	0.17	-1.50	2.70	1.93	1.42
	O89	N64	0.15	-1.16	2.71	1.90	1.41
	N79	O57	0.15	-1.01	2.68	1.42	1.94
	N49	O29	0.14	-1.02	2.86	1.40	1.91
$(EAN)_8$	O117	N109	0.19	-1.70	2.70	1.92	1.44
	O102	N94	0.19	-1.70	2.70	1.92	1.44
	O42	N34	0.18	-1.58	2.70	1.92	1.46
	O12	N4	0.18	-1.58	2.70	1.92	1.45
	O87	N79	0.17	-1.52	2.70	1.93	1.44
	O27	N19	0.17	-1.51	2.69	1.93	1.43
	O57	N49	0.17	-1.50	2.70	1.93	1.44
	O72	N64	0.17	-1.51	2.70	1.93	1.43
	N94	O72	0.15	-1.11	2.68	1.42	1.94
	N19	O12	0.15	-1.05	2.69	1.41	1.94
	N49	O42	0.13	-0.87	2.81	1.37	1.96
	N109	O87	0.13	-0.83	2.82	1.37	1.96
	N64	O27	0.12	-0.77	2.70	1.39	1.96
	N49	O29	0.12	-0.70	2.90	1.37	1.90
	N79	O57	0.12	-0.47	2.89	1.36	1.90
	N109	O104	0.11	-0.47	2.83	1.36	1.90
	N109	O104	0.09	-0.44	2.83	1.36	1.98

Table S3.2. Atoms participating in bonding interactions (Atom1 and Atom2), bond orders (BO), KBOs (kcal/mol) of the $N\cdots O$ interactions in $(EAN)_{10}$. Atom numbers in Atom1 and Atom2 are labeled in Figure 2f. The $N\cdots O$ distances (R) are in Å. Occ (Atom1) and Occ (Atom2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R(Å)	Occ (Atom1)	Occ (Atom2)
$(EAN)_{10}$	O147	N139	0.20	-1.80	2.70	1.91	1.46
	O132	N124	0.20	-1.78	2.70	1.91	1.45
	O42	N34	0.18	-1.60	2.70	1.92	1.46
	O117	N109	0.18	-1.56	2.70	1.92	1.45
	O27	N19	0.18	-1.53	2.68	1.93	1.44
	O87	N79	0.18	-1.53	2.69	1.93	1.44
	O12	N4	0.18	-1.53	2.70	1.93	1.43
	O72	N64	0,18	-1.55	2.70	1.93	1.42
	O57	N49	0.17	-1.53	2.68	1.93	1.43
	O102	N94	0.17	-1.51	2.70	1.93	1.44
	N19	O12	0.15	-1.47	2.70	1.41	1.95
	N79	O57	0.15	-1.09	2.89	1.40	1.94
	N124	O102	0.15	-1.05	2.83	1.41	1.95
	N49	O30	0.15	-0.99	2.83	1.38	1.91
	N49	O42	0.15	-1.03	2.89	1.39	1.95
	N94	O72	0.14	-0.89	2.90	1.41	1.95
	N109	O105	0.10	-0.41	2.89	1.36	1.91
	O44	N4	0.09	-0.50	2.90	1.98	1.35
	O150	N4	0.08	-0.37	2.89	1.98	1.38

Table S3.3. Atoms participating in bonding interactions (Atom1 and Atom2), bond orders (BO), KBOs (kcal/mol) of the $N\cdots O$ interactions in $(EAN)_{12}$. Atom numbers in Atom1 and Atom2 are labeled in Figure 2g. The $N\cdots O$ distances (R) are in Å. Occ (Atom1) and Occ (Atom2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R(Å)	Occ (Atom1)	Occ (Atom2)
$(EAN)_{12}$	O177	N169	0.20	-1.84	2.70	1.91	1.46
	O132	N124	0.19	-1.66	2.70	1.92	1.44
	O162	N154	0.19	-1.65	2.68	1.92	1.44
	O72	N64	0.18	-1.61	2.70	1.92	1.44
	O102	N94	0.18	-1.58	2.70	1.92	1.45
	O12	N4	0.18	-1.52	2.68	1.92	1.46
	O87	N79	0.18	-1.53	2.70	1.92	1.46
	O42	N34	0.18	-1.59	2.70	1.92	1.43
	O117	N109	0.18	-1.59	2.70	1.92	1.44
	O27	N19	0.17	-1.47	2.83	1.92	1.46
	N154	O14	0.16	-1.38	2.83	1.42	1.92
	N139	O117	0.15	-1.30	2.90	1.41	1.94
	O150	N124	0.13	-0.81	2.89	1.91	1.39
	N169	O45	0.12	-0.65	2.83	1.36	1.91
	N79	O57	0.11	-0.59	2.83	1.37	1.96
	N139	O104	0.10	-0.44	2.90	1.39	1.91
	N94	O42	0.09	-0.39	2.90	1.35	1.97
	N139	O102	0.08	-0.25	2.89	1.39	1.97
	N94	O44	0.08	-0.39	2.90	1.37	1.98
	O135	N109	0.08	-0.42	2.86	1.98	1.35
	N139	O104	0.08	-0.37	2.91	1.39	1.98
	N109	O72	0.07	-0.33	2.90	1.40	1.98

Table S3.4. Atoms participating in bonding interactions (Atom1 and Atom2), bond orders (BO), KBOs (kcal/mol) of the $N\cdots O$ interactions in $(EAN)_{16}$. Atom numbers in Atom1 and Atom2 are labeled in Figure 2h. The $N\cdots O$ distances (R) are in Å. Occ (Atom1) and Occ (Atom2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R(Å)	Occ (Atom1)	Occ (Atom2)
$(EAN)_{16}$	O 12	N4	0.19	-1.65	2.70	1.91	1.45
	O237	N229	0.19	-1.69	2.70	1.92	1.44
	O102	N94	0.19	-1.69	2.68	1.92	1.44
	O42	N34	0.19	-1.65	2.70	1.92	1.45
	O147	N139	0.18	-1.63	2.70	1.92	1.45
	O222	N214	0.18	-1.59	2.68	1.92	1.43
	O117	N109	0.18	-1.58	2.70	1.92	1.42
	O27	N19	0.18	-1.53	2.70	1.92	1.45
	O162	N154	0.18	-1.56	2.68	1.93	1.44
	O132	N124	0.17	-1.50	2.70	1.92	1.46
	O72	N64	0.18	-1.61	2.70	1.92	1.46
	O192	N184	0.18	-1.52	2.68	1.92	1.42
	O87	N79	0.18	-1.55	2.70	1.93	1.44
	O177	N169	0.18	-1.50	2.70	1.93	1.43
	N229	O207	0.18	-1.47	2.70	1.44	1.44
	O57	N49	0.17	-1.45	2.70	1.93	1.43
	N94	O74	0.17	-1.48	2.80	1.43	1.90
	N184	O162	0.15	-1.15	2.85	1.40	1.95
	N169	O147	0.15	-1.11	2.89	1.40	1.95
	N79	O57	0.14	-0.97	2.83	1.41	1.95
	N199	O177	0.13	-0.83	2.90	1.39	1.96
	N64	O27	0.12	-0.73	2.89	1.40	1.96
	N109	O102	0.11	-0.58	2.83	1.39	1.96

4. List of unique QUAOs for the $(EAN)_1$:$(1\text{-}AT)_n$ (n=1-5)

Table S4.1. Average Bond orders, KBOs (kcal/mol) of the N···O interactions for $(EAN)_1$:$(1\text{-}AT)_n$ (n =1 – 5). N···O distances (R_{NO}) are in Å for $(EAN)_1$:$(1\text{-}AT)_n$ (n =1 – 5).

Systems	R_{NO} (Å)	BO	KBO (kcal/mol)
$(EAN)_1$:$(1\text{-}AT)_1$	2.75	0.15	-1.74
$(EAN)_1$:$(1\text{-}AT)_2$	2.80	0.15	-1.70
$(EAN)_1$:$(1\text{-}AT)_3$	2.82	0.12	-1.64
$(EAN)_1$:$(1\text{-}AT)_4$	2.82	0.12	-1.67
$(EAN)_1$:$(1\text{-}AT)_5$	2.85	0.11	-1.68

Table S4.2. Average Bond orders, KBOs (kcal/mol) of the Ethylammonium N···N (1-AT) interactions for $(EAN)_1$:$(1\text{-}AT)_n$ (n =1 – 5). Ethylammonium N···N (1-AT) distances (R_{NN}) are in Å

Systems	R_{NN} (Å)	BO	KBO (kcal/mol)
$(EAN)_1$:$(1\text{-}AT)_1$	2.74	0.07	-0.18
$(EAN)_1$:$(1\text{-}AT)_2$	2.98	0.10	-0.42
$(EAN)_1$:$(1\text{-}AT)_3$	-	-	-
$(EAN)_1$:$(1\text{-}AT)_4$	2.86	0.13	-0.76
$(EAN)_1$:$(1\text{-}AT)_5$	2.80	0.19	-1.46

Table S4.3. Atoms participating in bonding interactions (Atom1 and Atom2), bond orders (BO), KBOs (kcal/mol) for the H-bonds in $(EAN)_1$:$(1\text{-}AT)_n$ (n=1-5). Atom numbers in Atom1 and Atom2 are labeled in Figure 3. R represents the H-bond distance in Å. Occ (Atom1) and Occ (Atom 2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively. Orbital (Atom1) and Orbital (Atom2) are types of orbitals in Atom1 and Atom2 participating in the H-bonding interactions, respectively. The KBO in parentheses is the sum of H-bonding interactions with $N\cdots O$ and $N\cdots N$ KBO.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R (Å)	Occ (Atom1)	Orbital (Atom 1)	Occ (Atom2)	Orbital (Atom2)
$(EAN)_1$:$(1\text{-}AT)_1$	O12	H5	0.33	-5.11 (-6.77)	1.82	1.92	*p*l	0.61	*σ*
	H22	O12	0.10	-1.91 (-2.73)	2.14	0.67	*σ*	1.96	*pl*
	N17	H5	0.11	-0.69 (-0.87)	2.17	1.99	*p*l	0.61	*σ*
$(EAN)_1$:$(1\text{-}AT)_2$	O12	H5	0.30	-5.13 (-6.83)	1.75	1.92	*p*l	0.62	*σ*
	H32	O14	0.16	-1.77 (-2.41)	1.98	0.69	*σ*	1.90	*pl*
	N18	H6	0.15	-0.98 (-1.40)	2.22	1.94	*p*l	0.65	*σ*
$(EAN)_1$:$(1\text{-}AT)_3$	O12	H5	0.30	-5.06 (-6.74)	1.75	1.92	*p*l	0.62	*σ*
	H32	O15	0.17	-1.91 (-2.65)	1.99	0.69	*σ*	1.91	*pl*
	H42	N18	0.18	-1.67 (-2.37)	2.09	0.70	*σ*	1.93	*pl*
	H22	O12	0.13	-0.97 (-1.45)	2.09	0.69	*σ*	1.97	*pl*
	H22	O12	0.11	-0.74 (-0.96)	2.09	0.69	*σ*	1.82	*pl*
$(EAN)_1$:$(1\text{-}AT)_4$	O12	H5	0.27	-4.60 (-6.12)	1.75	1.93	*p*l	0.63	*σ*
	N48	H6	0.27	-3.80 (-5.14)	1.87	1.91	*pl*	0.65	*σ*
	H22	O12	0.15	-1.41 (-2.02)	2.03	0.69	*σ*	1.95	*pl*
	H33	O12	0.13	-0.97 (-1.37)	2.06	0.69	*σ*	1.95	*pl*
	N17	H5	0.11	-0.76 (-0.95)	2.17	1.96	*pl*	0.63	*σ*
$(EAN)_1$:$(1\text{-}AT)_5$	O12	H5	0.27	-4.63 (-6.14)	1.75	1.93	*p*l	0.63	*σ*
	N48	H6	0.29	-4.11 (-5.57)	1.86	1.90	*pl*	0.66	*σ*
	H22	O12	0.15	-1.31 (-1.88)	2.03	0.69	*σ*	1.96	*pl*
	H33	O14	0.11	-0.81 (-1.09)	2.09	0.70	*σ*	1.91	*pl*
	H42	O15	0.10	-0.66 (-0.24)	2.09	0.69	*σ*	1.92	*pl*

5. List of unique QUAOs for the $(EAN)_2$:$(1\text{-}AT)_n$ (n=1-5)

Table S5.1. Average Bond orders and KBOs (kcal/mol) of the Ethylammonium N···O (Nitrate) interactions for $(EAN)_2$:$(1\text{-}AT)_n$ (n =1 – 5). The Ethylammonium N···O (Nitrate) distances (R_{NO}) are in Å

Systems	R_{NO} (Å)	BO	KBO (kcal/mol)
$(EAN)_2$:$(1\text{-}AT)_1$	2.70	0.18	-1.63
$(EAN)_2$:$(1\text{-}AT)_2$	2.70	0.15	-1.20
$(EAN)_2$:$(1\text{-}AT)_3$	2.74	0.15	-1.19
$(EAN)_2$:$(1\text{-}AT)_4$	2.74	0.13	-0.98
$(EAN)_2$:$(1\text{-}AT)_5$	2.78	0.12	-0.96

Table S5.2. Average Bond orders and KBOs (kcal/mol) of the 1-AT N···O (Nitrate) interactions for $(EAN)_2$:$(1\text{-}AT)_n$ (n =1 – 5). 1-AT N···O (Nitrate) distances (R_{NO}) are in Å

Systems	R_{NO} (Å)	BO	KBO (kcal/mol)
$(EAN)_2$:$(1\text{-}AT)_1$	2.95	0.10	-0.49
$(EAN)_2$:$(1\text{-}AT)_2$	2.95	0.10	-0.51
$(EAN)_2$:$(1\text{-}AT)_3$	2.96	0.10	-0.56
$(EAN)_2$:$(1\text{-}AT)_4$	2.97	0.11	-0.61
$(EAN)_2$:$(1\text{-}AT)_5$	2.98	0.10	-0.63

Table S5.3. Average Bond orders and KBOs (kcal/mol) of the Ethylammonium N···N (1-AT) interactions for $(EAN)_2$:$(1\text{-}AT)_n$ (n =1 – 5). Ethylammonium N···N (1-AT) distances (R_{NN}) are in Å.

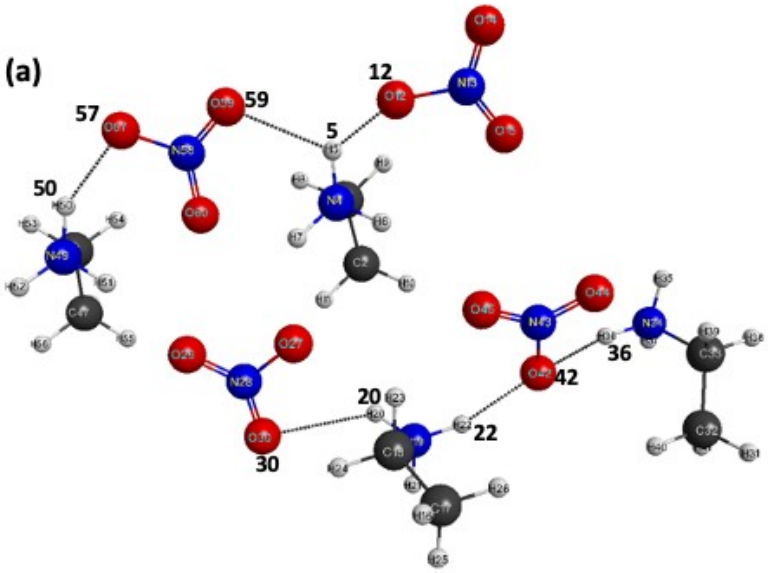
Systems	R_{NN} (Å)	BO	KBO (kcal/mol)
$(EAN)_2$:$(1\text{-}AT)_1$	2.99	0.11	-0.45
$(EAN)_2$:$(1\text{-}AT)_2$	2.97	0.13	-0.32
$(EAN)_2$:$(1\text{-}AT)_3$	3.02	0.10	-0.39
$(EAN)_2$:$(1\text{-}AT)_4$	3.02	0.12	-0.70
$(EAN)_2$:$(1\text{-}AT)_5$	2.93	0.16	-1.07

Table S5.4. Atoms participating in bonding interactions (Atom1 and Atom2), bond orders (BO), KBOs (kcal/mol) for the H-bonds in $(EAN)_2$:$(1\text{-}AT)_n$ (n=1-5). Atom numbers in Atom1 and Atom2 are labeled in Figure 4. R represents the H-bond distance in Å. Occ (Atom1) and Occ (Atom2) are occupations of the QUAOs centered on Atom1 and Atom2, respectively. Orbital (Atom1) and Orbital (Atom2) are types of orbitals in Atom1 and Atom2 participating in the H-bonding interactions, respectively. The KBO in parentheses is the sum of H-bonding interactions with $N\cdots O$ and $N\cdots N$ KBOs.

System	Atom1	Atom2	BO	KBO (kcal/mol)	R (Å)	Occ (Atom1)	Orbital (Atom1)	Occ (Atom2)	Orbital (Atom2)
$(EAN)_2$:$(1\text{-}AT)_1$	O 12	H 5	0.29	-5.04 (-6.67)	1.75	1.92	*p*l	0.61	*σ*
	O 27	H 20	0.29	-4.99 (-6.62)	1.75	1.92	*p*l	0.62	*σ*
	N 33	H 22	0.15	-1.03 (-1.49)	2.13	1.94	*p*l	0.66	*σ*
	H 37	O 12	0.14	-1.17 (-1.66)	2.17	0.68	*σ*	1.97	*pl*
	O 29	H 7	0.12	-0.82 (-1.21)	2.68	1.98	*p*l	0.65	*σ*
$(EAN)_2$:$(1\text{-}AT)_2$	O12	H5	0.29	-5.05 (-6.69)	1.75	1.92	*p*l	0.62	*σ*
	O27	H20	0.29	-4.96 (-6.58)	1.75	1.92	*p*l	0.62	*σ*
	N43	H22	0.16	-1.28 (-1.60)	2.09	1.94	*p*l	0.66	*σ*
	O 29	H 7	0.13	-1.18 (-3.40)	1.97	1.91	*p*l	0.66	*σ*
	H47	O12	0.14	-1.20 (-1.71)	2.17	0.68	*σ*	1.97	*σ*
$(EAN)_2$:$(1\text{-}AT)_3$	O12	H5	0.29	-5.09 (-6.75)	1.75	1.92	*p*l	0.62	*σ*
	O27	H20	0.28	-4.63 (-6.16)	1.75	1.93	*p*l	0.62	*σ*
	H47	O12	0.15	-1.32 (-1.88)	2.15	0.68	*σ*	1.97	*pl*
	O29	H7	0.14	-1.25 (-1.62)	1.95	1.91	*p*l	0.66	*σ*
	N43	H22	0.14	-0.90 (-1.30)	3.00	1.94	*p*l	0.66	*σ*
$(EAN)_2$:$(1\text{-}AT)_4$	O12	H5	0.28	-4.85 (-6.45)	1.75	1.93	*p*l	0.63	*σ*
	O27	H20	0.28	-4.68 (-6.23)	1.75	1.93	*p*l	0.62	*σ*
	N62	H6	0.22	-2.68 (-3.72)	2.00	1.93	*p*l	0.67	*σ*
	H47	O12	0.15	-1.41 (-2.01)	2.14	1.91	*pl*	1.97	*σ*
	H67	O15	0.11	-0.79 (-1.19)	2.11	0.69	*σ*	1.98	*pl*
	O29	H7	0.11	-0.78 (-1.17)	1.98	0.69	*σ*	0.67	*pl*
	N43	H22	0.13	-0.78 (-1.13)	2.19	1.96	*pl*	0.66	*σ*
$(EAN)_2$:$(1\text{-}AT)_5$	O12	H5	0.28	-4.85 (-6.45)	1.75	1.92	*p*l	0.63	*σ*
	O27	H20	0.28	-4.74 (-6.32)	1.92	1.92	*pl*	0.63	*σ*
	N43	H22	0.25	-3.08 (-4.21)	2.03	1.92	*p*l	0.66	*pl*
	N76	H6	0.24	-2.77 (-3.83)	2.03	1.93	*pl*	0.67	*pl*
	N52	O21	0.20	-2.66 (-3.69)	2.00	1.93	*pl*	0.66	*pl*
	H67	O12	0.15	-1.39 (-2.02)	2.03	0.69	*σ*	1.96	*σ*
	H47	O14	0.14	-1.15 (-1.19)	1.92	0.68	*σ*	1.98	*sl*
	H47	O14	0.13	-1.18 (-1.51)	1. 92	0.68	*σ*	1.91	*pl*
	O29	H7	0.13	-1.11 (-3.34)	1.99	1.91	*σ*	0.66	*σ*

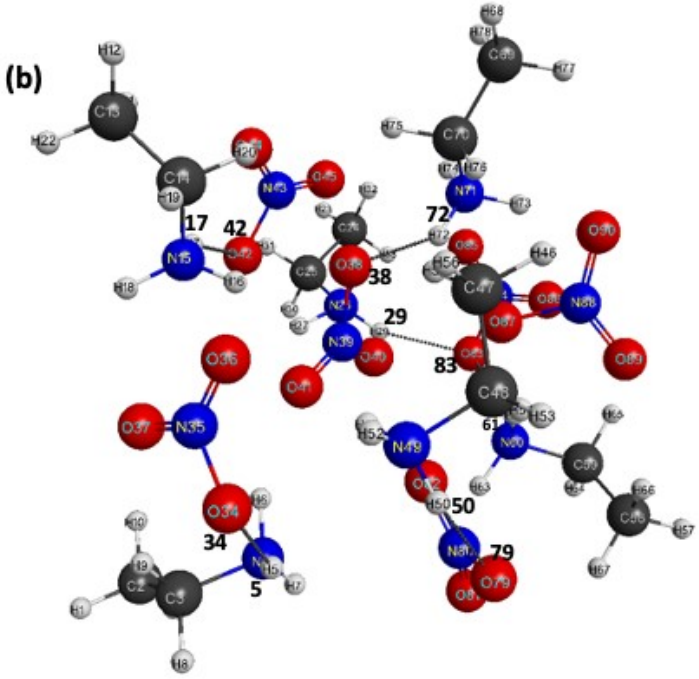
List of low energy geometries for $(EAN)_n$ (n=4,8,10,16,24)

(a)



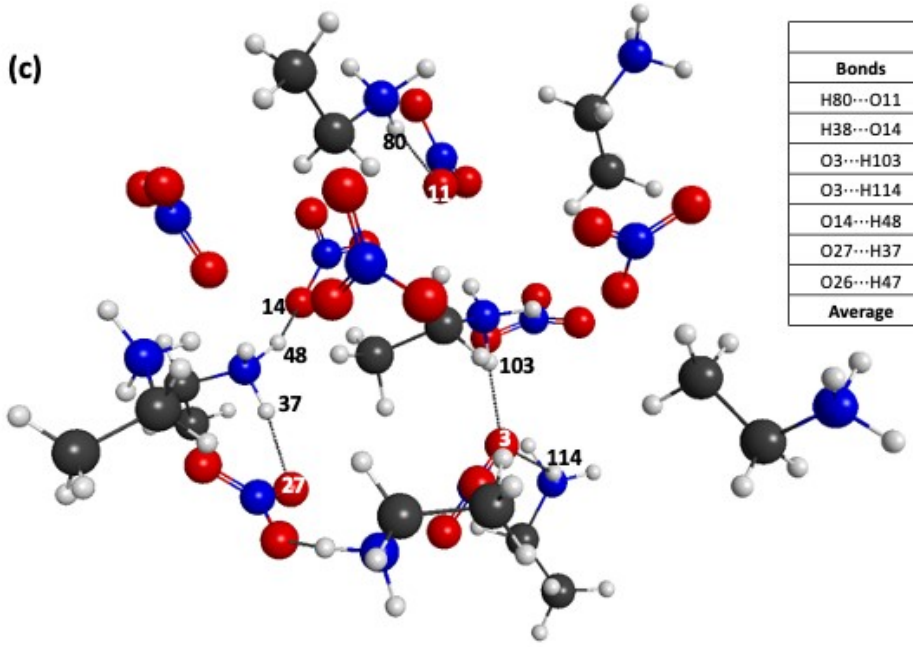
$(EAN)_4$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
H5···O12	1.75	155.99
H5···O59	2.22	144.47
O57···H50	1.75	155.99
O30···H20	1.75	155.99
O42···H36	1.75	155.99
O42···H22	1.85	163.66
Average	**1.86 Å**	**155.22 °**

(b)



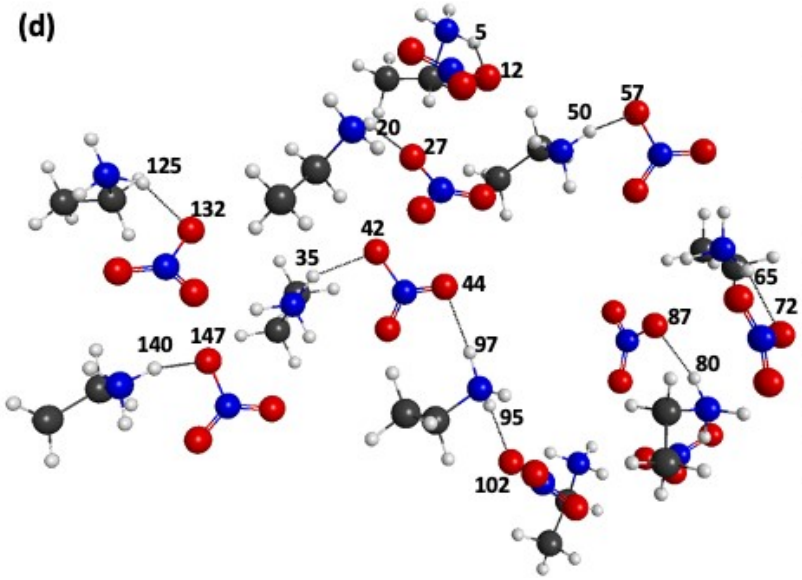
$(EAN)_6$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
H17···O42	1.75	155.99
H5···O34	2.22	144.47
O79···H50	1.75	155.99
O83···H29	1.75	155.99
O38···H72	1.75	155.99
O83···H61	1.93	167.43
Average	**1.86 Å**	**155.97 °**

(c)



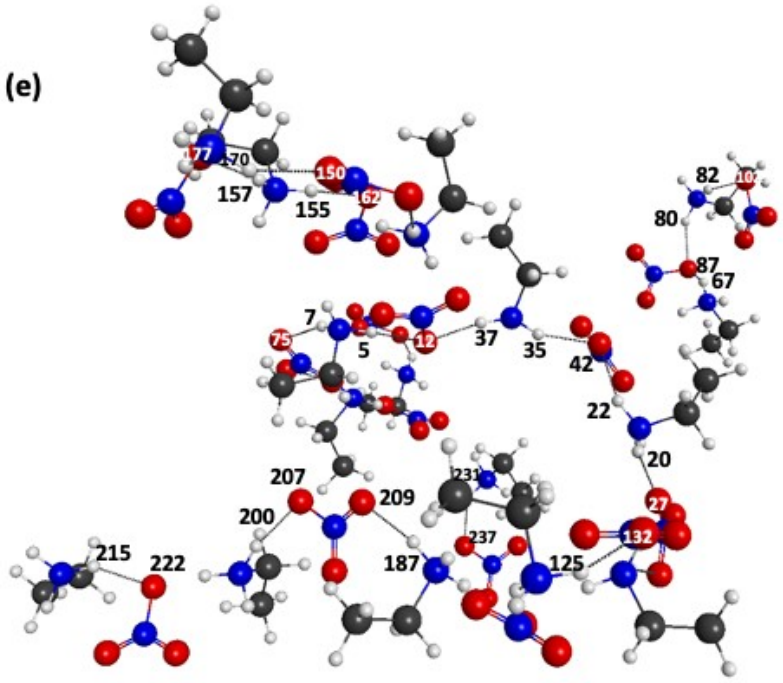
$(EAN)_8$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
H80···O11	1.75	155.99
H38···O14	1.75	115.94
O3···H103	1.75	155.99
O3···H114	1.83	140.40
O14···H48	1.75	155.99
O27···H37	1.86	164.38
O26···H47	1.75	155.99
Average	**1.78 Å**	**149.24 °**

(d)



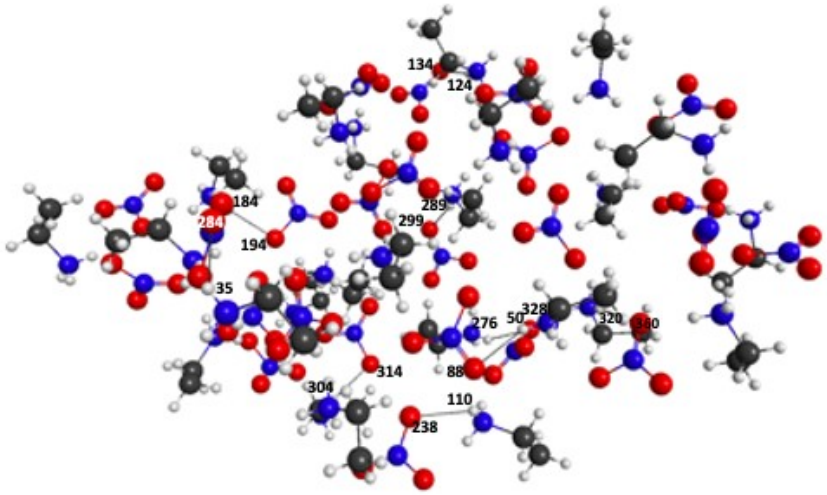
$(EAN)_{10}$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
H125···O132	1.75	155.99
H140 ···O147	1.75	155.99
O42 ···H35	1.75	155.99
O44 ···H97	1.93	169.44
O27 ···H20	1.75	155.99
O102 ···H95	1.75	155.99
O12···H5	1.75	155.99
H5···O12	1.75	155.99
H50 ···O57	1.75	155.99
H65···O72	1.93	155.79
H80···O87	1.83	157.07
Average	**1.88Å**	**157.29 °**

(e)



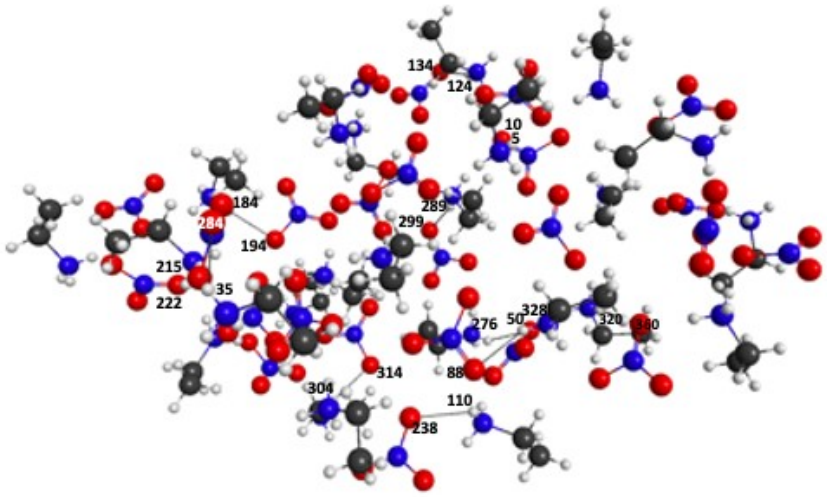
$(EAN)_{16}$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
H5···O12	1.90	149.47
H75···O147	1.75	155.99
O27···H35	1.75	155.99
O42···H97	1.93	169.44
O42···H20	1.75	155.99
O12···H37	1.75	155.99
O12···H5	1.75	155.99
H5···O12	1.75	155.99
H50 ···O57	1.75	155.99
H65···O72	1.93	155.79
H67···O87	1.78	157.07
H80···O87	1.88	149.52
H82···O102	1.75	152.84
H80···O87	1.88	155.79
O132···H125	1.75	156.22
O162···H155	1.86	162.47
O157···H177	1.85	150.52
O150···H170	1.86	151.70
O209···H187	1.86	167.43
O207···H200	1.87	159.30
O222···H215	1.82	145.67
O237···H231	1.75	155.99
Average	**1.81Å**	**155.96 °**

(f)



$(EAN)_{24}$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
O134···H124	2.10	164.22
O284···H35	2.01	164.22
O238···H110	1.94	155.99
O360···H320	2.22	112.25
O314···H304	2.07	164.22
O328···H276	1.75	155.99
O88···H50	2.08	148.98
O299···H289	2.10	164.22
O194···H184	2.07	164.22
Average	**2.04Å**	**154.92 °**

(g)

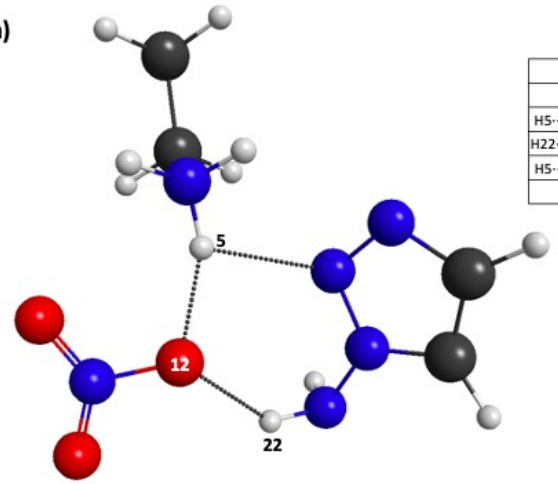


$(EAN)_{24}$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
O134···H124	2.10	164.22
O284···H35	2.01	164.22
O238···H110	1.94	155.99
O360···H320	2.22	112.25
O314···H304	2.07	164.22
O328···H276	1.75	155.99
O88···H50	2.08	148.98
O299···H289	2.10	164.22
O194···H184	2.07	164.22
O10···H5	1.75	155.99
O222···H215	2.10	164.22
Average	**2.02Å**	**155.9 ***

*Lowest energy geometry

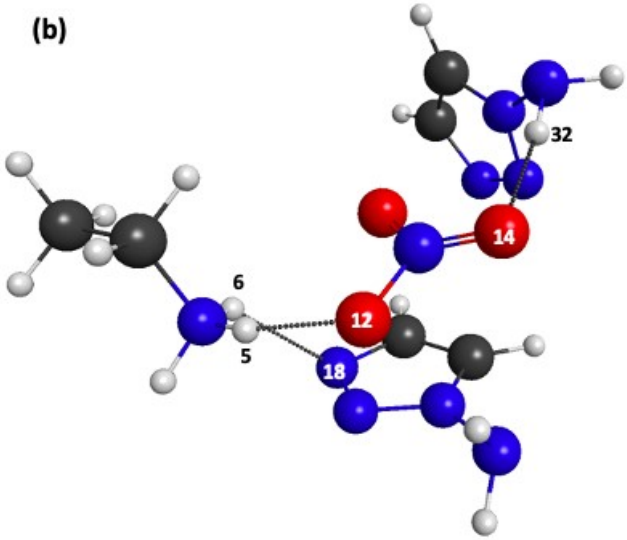
Figure S1. The second lowest energy geometry from EFP MC sampled geometries for (a) $(EAN)_4$ (b) $(EAN)_{6,}$ (c) $(EAN)_8$, (d) $(EAN)_{10}$ (e) $(EAN)_{16}$ (f) $(EAN)_{24}$ and EFP MC optimized lowest energy geometry for (g) $(EAN)_{24}$. Atoms that have H-bonding interactions are indicated by atom numbers and listed under "Bonds". Hydrogen bonds are indicated with dotted lines. R_{H-bond} represents the distance between a hydrogen atom from $[EA]^+$ and an oxygen atom from $[NO_3]^-$ that form a H-bond. Units are in Å. Θ_{H-bond} is the angle measured in ethylammonium N-H ···O (nitrate).

(a)



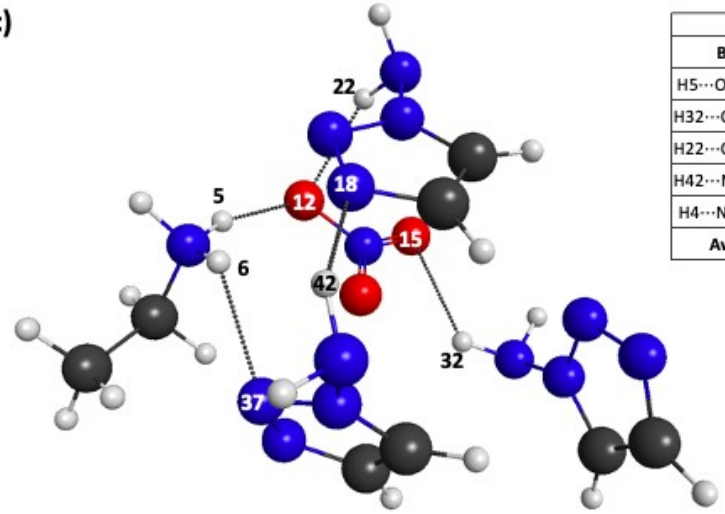
$(EAN)_1$:(1-AT)$_1$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
H5···O12 (sd,da)	1.75	155.99
H22···O12 (sd,da)	2.02	137.34
H5···N17 (sd,da)	2.17	89.95
Average	**1.98 Å**	**127.76 °**

(b)

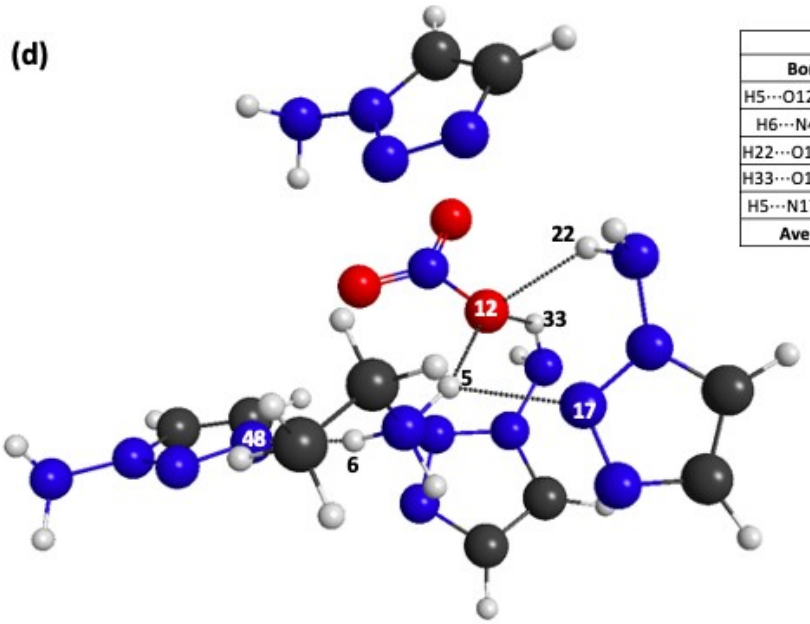


$(EAN)_1$:(1-AT)$_2$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
H5···O12 (dd,sa)	1.75	155.99
H32···O14 (sd,sa)	1.98	171.99
H6···N18 (dd,sa)	2.22	130.58
Average	**1.98 Å**	**152.85 °**

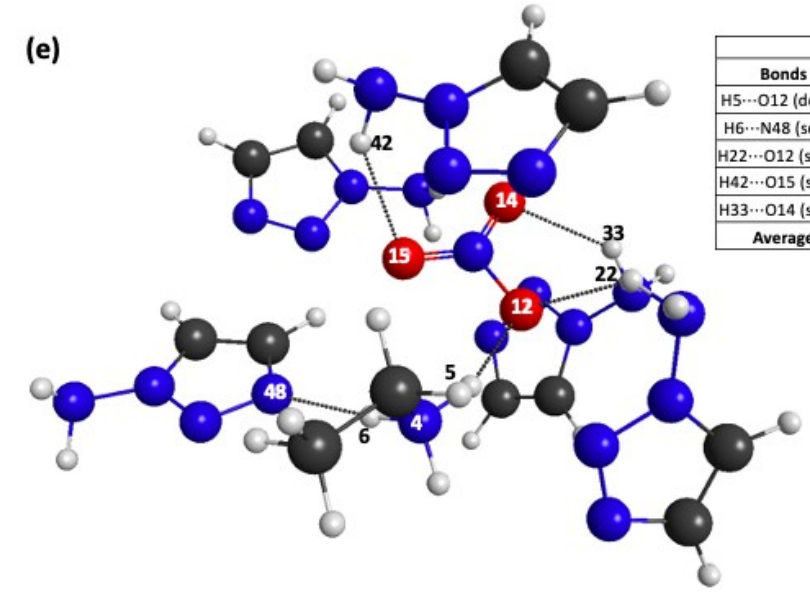
(c)



$(EAN)_1$:(1-AT)$_3$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
H5···O12 (dd,da)	1.75	155.99
H32···O15 (sd,da)	1.99	173.92
H22···O12 (sd,da)	2.09	135.30
H42···N18 (sd,da)	2.09	138.07
H4···N37 (dd,sa)	2.33	134.45
Average	**2.05 Å**	**147.55 °**



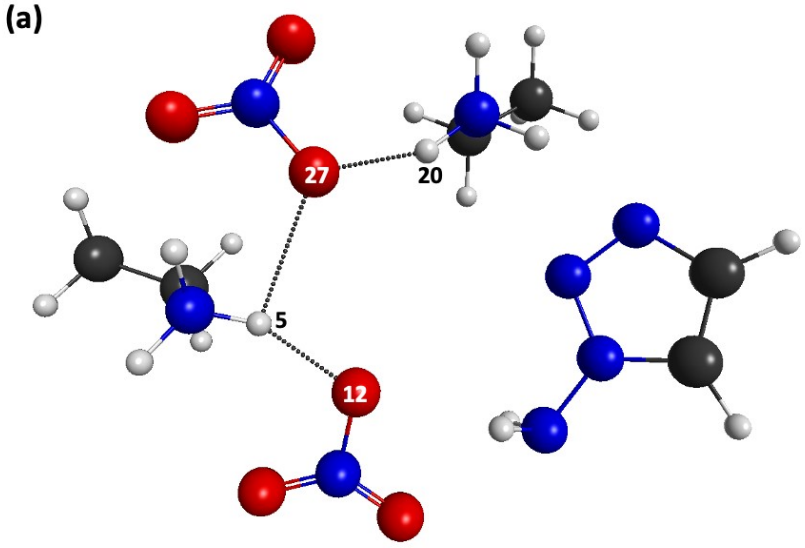
$(EAN)_1$:$(1\text{-}AT)_4$		
Bonds	R_{H-bond}(Å)	Θ_{H-bond}(Degree)
H5···O12 (dd,da)	1.75	155.99
H6···N48 (dd)	1.87	164.24
H22···O12 (sd.da)	2.03	137.30
H33···O12 (sd,da)	2.06	133.97
H5···N17 (dd,sa)	2.17	113.57
Average	**1.98 Å**	**141.01 °**



$(EAN)_1$:$(1\text{-}AT)_5$		
Bonds	R_{H-bond}(Å)	Θ_{H-bond}(Degree)
H5···O12 (dd,da)	1.75	155.99
H6···N48 (sd,sa)	1.86	162.12
H22···O12 (sd,da)	2.03	135.82
H42···O15 (sd,sa)	2.09	139.09
H33···O14 (sd,sa)	2.09	138.92
Average	**1.96 Å**	**146.39 °**

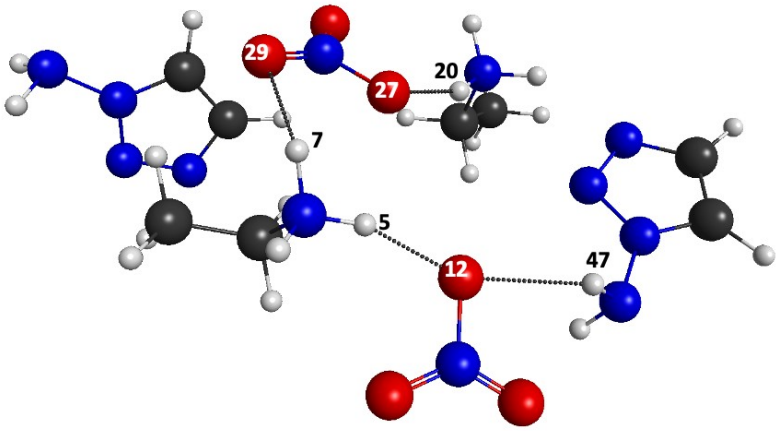
Figure S2. The second lowest energy geometry from EFP MC sampled geometries for $(EAN)_1$:$(1\text{-}AT)_n$ (n=1-5). Atoms that have H-bonding interactions are indicated by atom numbers and listed under "Bonds". Hydrogen bonds are indicated with dotted lines. R_{H-bond} represents the distance between a hydrogen atom from $[EA]^+$ and an oxygen atom from $[NO_3]^-$ that form a H-bond. Units are in Å. Θ_{H-bond} is the angle measured in ethylammonium N-H···O (nitrate).

(a)



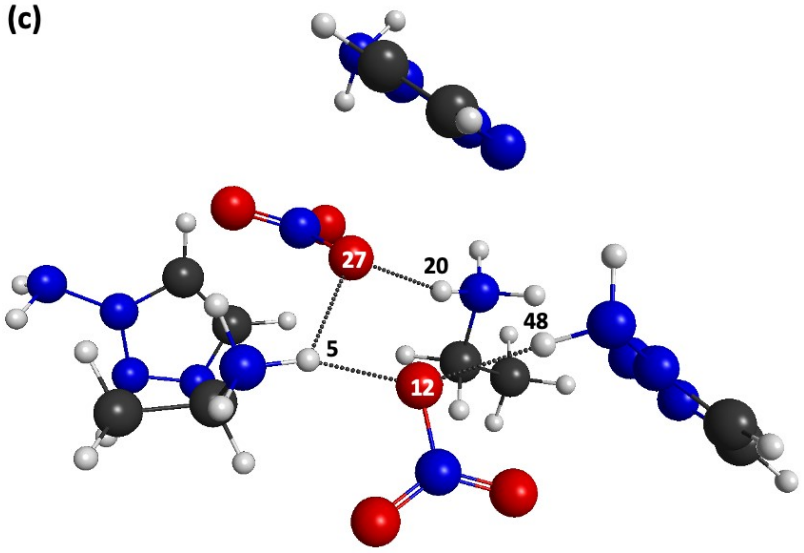
$(EAN)_2$:(1-AT)$_1$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
H5···O12	1.75	155.99
H5-O27	2.35	98.06
O27-H20	1.75	155.99
Average	**1.95 Å**	**136.68 °**

(b)



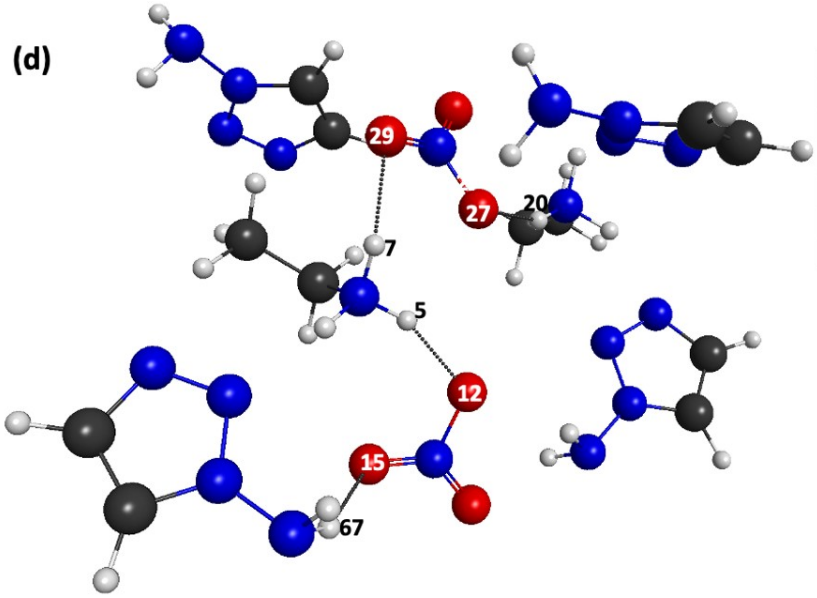
$(EAN)_2$:(1-AT)$_2$		
Bonds	**R_{H-bond}(Å)**	**Θ_{H-bond}(Degree)**
H5···O12	1.75	141.78
H47-O12	2.14	133.18
H7-O29	1.99	138.79
H20-O27	1.75	155.99
Average	**1.91 Å**	**142.44 °**

(c)

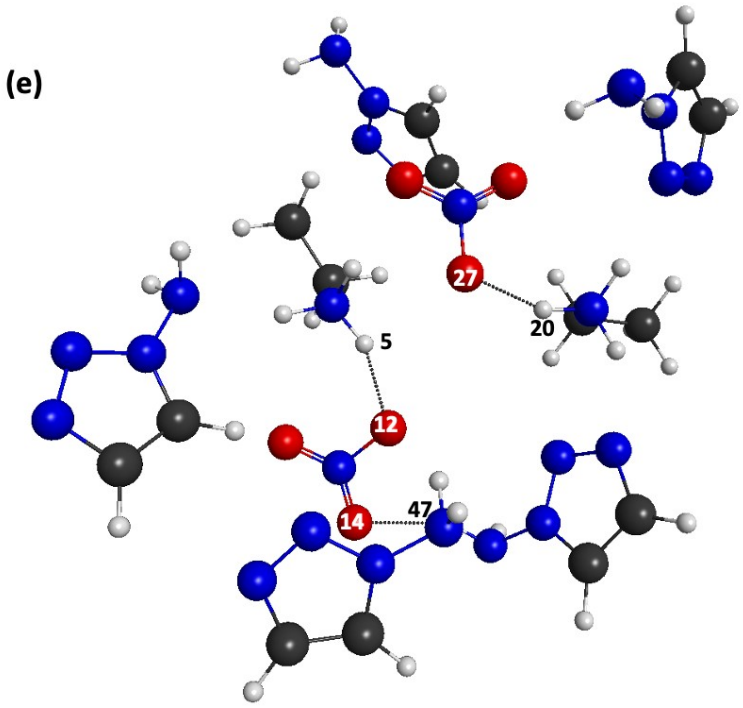


$(EAN)_2$:$(1\text{-}AT)_3$		
Bonds	$\mathbf{R_{H-bond}}$**(Å)**	$\mathbf{\Theta_{H-bond}}$**(Degree)**
H5···O12	1.75	155.99
H5···O27	1.90	121.41
H20···O27	1.75	155.99
H48···O12	2.07	167.73
Average	**1.87 Å**	**150.28°**

(d)



$(EAN)_2$:$(1\text{-}AT)_4$		
Bonds	$\mathbf{R_{H-bond}}$**(Å)**	$\mathbf{\Theta_{H-bond}}$**(Degree)**
H5···O12	1.75	141.78
H7···O29	1.86	157.29
H20···O27	1.75	155.99
H67···O15	2.13	151.15
Average	**1.87 Å**	**151.55 °**



$(EAN)_2$:$(1\text{-}AT)_5$		
Bonds	$\mathbf{R_{H-bond}}$**(Å)**	$\mathbf{\Theta_{H-bond}}$**(Degree)**
H5···O12	1.75	155.99
H47···O14	1.90	144.47
H20···O27	1.12	165.4
Average	**1.59Å**	**155.29°**

Figure S3. The second lowest energy geometry from EFP MC sampled geometries for $(EAN)_2$:$(1\text{-}AT)_n$ (n=1-5). Atoms that have H-bonding interactions are indicated by atom numbers and listed under "Bonds". Hydrogen bonds are indicated with dotted lines. R_{H-bond} represents the distance between a hydrogen atom from $[EA]^+$ and an oxygen atom from $[NO_3]^-$ that form a H-bond. Units are in Å. Θ_{H-bond} is the angle measured in ethylammonium N-H···O (nitrate).