

Design tri-branched multiple-site SO₂ capture materials

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Supporting Information

Contents

Table S1	Calculated sequential SO ₂ binding energies of reported anions.....	3
Table S2	Calculated sequential SO ₂ binding energies of selected anions.....	4
Table S3	Detailed simulated capacities of selected anions.....	4
Figure S1	Other tri-branched species studied in this work.....	5
Figure S2	Configurations of selected anions and their sequential SO ₂ absorptions.....	5
Figure S3	Line chart of calculated sequential SO ₂ binding energies of the studied anions.....	6
Figure S4	Stacked column plot of calculated sequential SO ₂ binding energies of the studied anions.....	6
Figure S5	Configurations of the sequential SO ₂ absorptions using TIA	7
Figure S6	Various stable configurations of TAEA and SO ₂ complexes.....	7
Figure S7	The first binding energy of studied anions and SO ₂ versus the NBO orbital energy of the lone pair of the reacting N atom.....	9
Figure S8	The first binding energy of selected anions and SO ₂ versus the NBO orbital energy of the lone pair of the reacting N or S atom.....	9
Figure S9	Multiple-site interactions in the optimized structures based on Tetz and NO dimers.....	10
Figure S10	Multiple-site interactions in the optimized structures based on TAEA and NO dimers.....	10
Reference	11

TableS1. Calculated sequential SO₂ binding energies (kJ mol⁻¹) of reported anions. Sequential SO₂ interacting positions with **Tetz** are labeled by numbers in red.

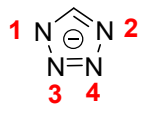
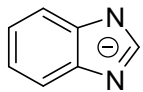
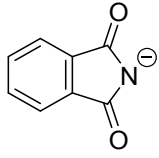
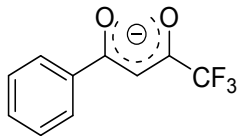
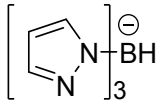
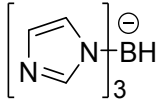
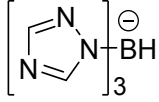
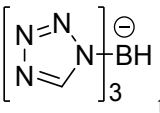

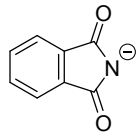
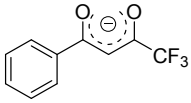
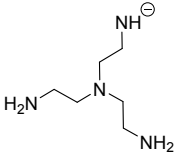
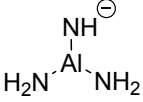
E _b	1	2	3	4	5	Ref
 Tetz	-89.3	-59.9	-39.7	-34.4	---	1
 BenIm	-98.2	-53.7	-19.6	---	---	2
 Phth	-68.7	-42.3	-39.5	-34.4	-30.9	3
 BTFA	-89.4	-60.6	-56.9	-54.7	---	4
 tri(imidazolyl)hydroborate	-56.9	-50.7	-46.5	---	---	5
 tri(pyrazolyl)hydroborate	-63.1	-56.2	-52.8	---	---	5
 tri(1,2,4-triazolyl)hydroborate	-49.1	-48.2	-42.1	-31.2	---	5
 tri(tetrazolyl)hydroborate	-37.6	-36.7	-34.7	-24.4	---	5

Table S2. Calculated sequential SO₂ binding energies (kJ mol⁻¹) of selected anions. “-n” means the neutral molecule of the anion counterpart shown in Figure 1.

E _b	TAA-n	TAMA-n	TAEA-n	TAAL-n	TIA-n	TIA-1-n	TIAL-n	TIAL-1-n	TAB-n
	n								
1	-26.5	-47.2	-46.8	-74.7	-27.6	-37.5	-27.3	-94.5	-26.2
2	-24.3	-34.2	-48.3	-57.7	-25.9	-33.2	-28.2	-72.2	-21.5
3	-21.3	-25.7	-46.3	-46.0	-25.0	-32.7	-32.9	-49.4	-16.7
E _b	TIB-n	TIB-1-n	TPA	TPB	TIA-2	TIAL-2	TIB-2	THMA	THB
1	-27.8	-36.1	-27.3	-32.1	-25.8	-25.8	-27.5	-148.4	-104.0
2	-27.2	-36.9	-28.5	-26.5	-24.7	-24.8	-26.7	-60.7	-67.3
3	-27.2	-35.1	-25.5	-14.8	-23.5	-24.1	-26.3	-43.8	-28.4

Table S3. Detailed simulated capacities of the selected anions.

Anions	Absorption capacity (1 bar of SO ₂ , 20°C)	Residual capacity (1 bar of SO ₂ , 120°C)	Available capacity
	3.44	1.91	1.53
	3.59	1.04	2.55
	4.00	3.38	0.62
	6.12	4.95	1.17
	5.96	4.10	1.86

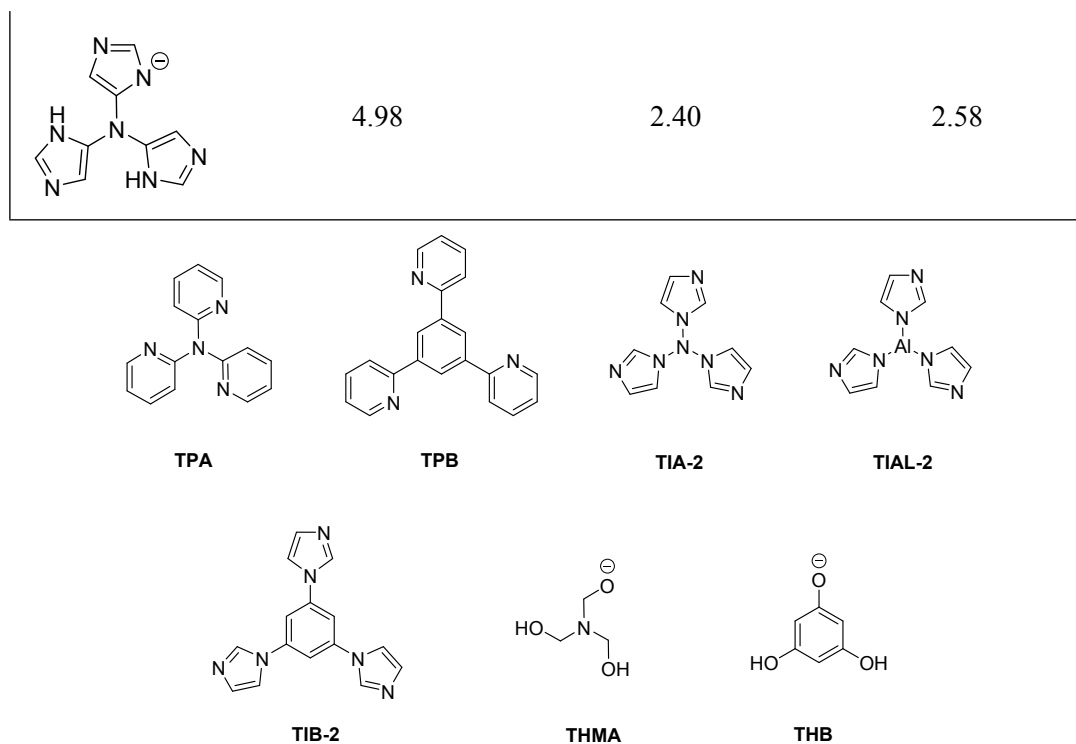


Figure S1. Other tri-branched species (including anion and neutral ones) studied in this work.

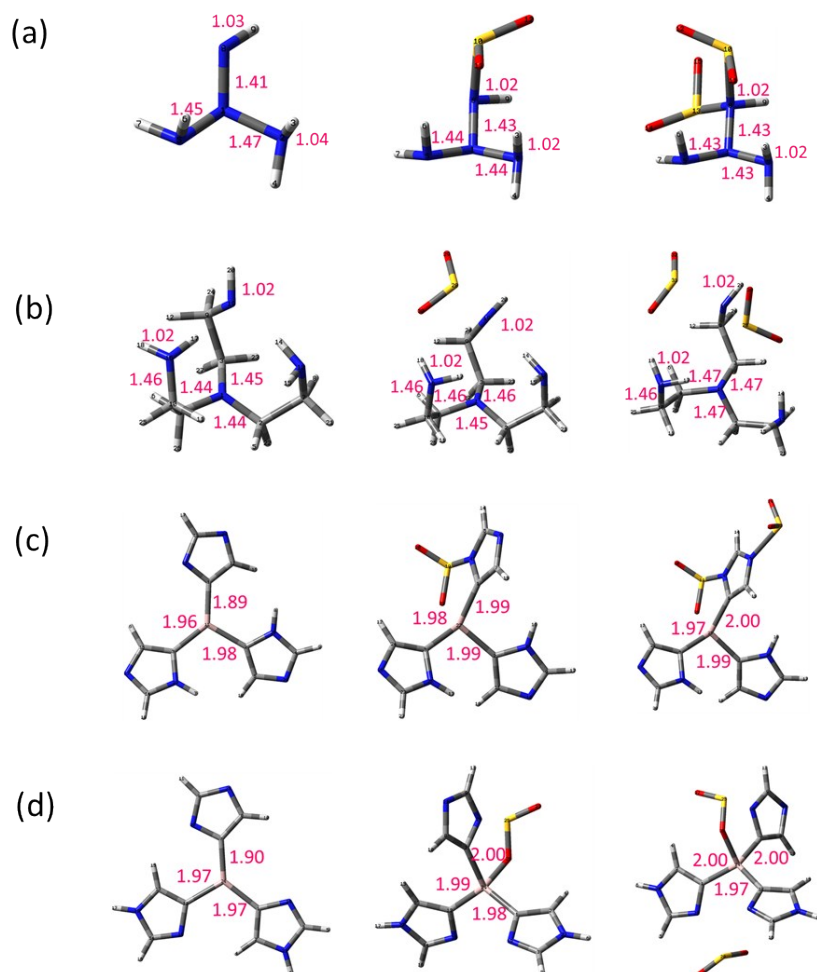


Figure S2. Configurations of (a) **TAA**, (b) **TAEA**, (c) **TIAL** and (d) **TIAL-1** with their sequential SO₂ absorptions. The important bond lengths (Å) are given. Red is oxygen, blue is nitrogen, yellow is sulfur, gray is carbon and white is hydrogen.

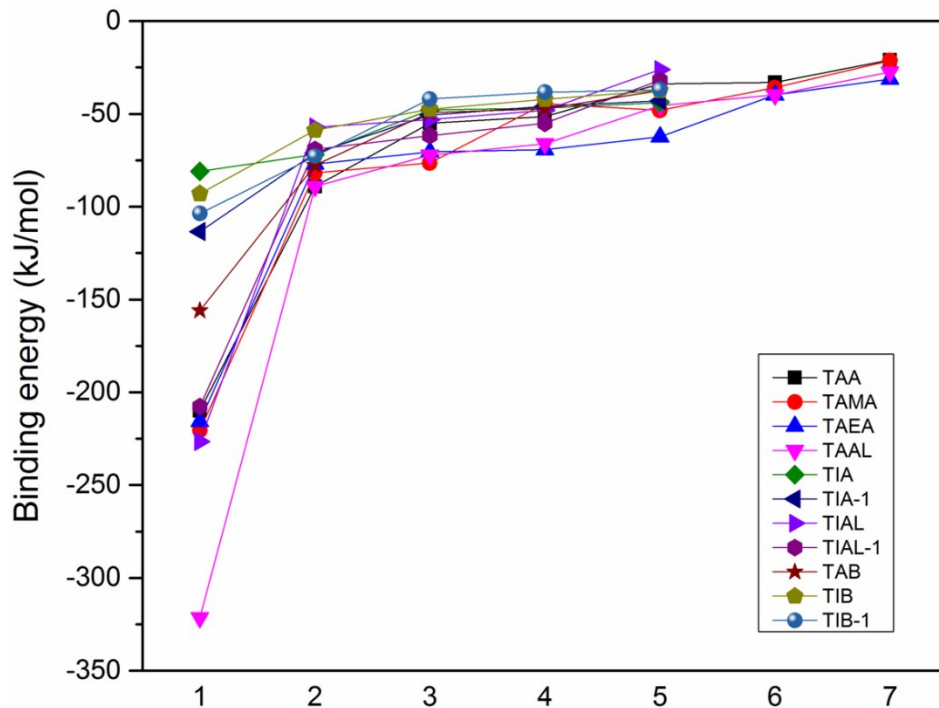


Figure S3. Line chart of calculated sequential SO_2 binding energies (kJ mol^{-1}) of the studied anions. Consecutive numbers below means the numbers of absorbed SO_2 .

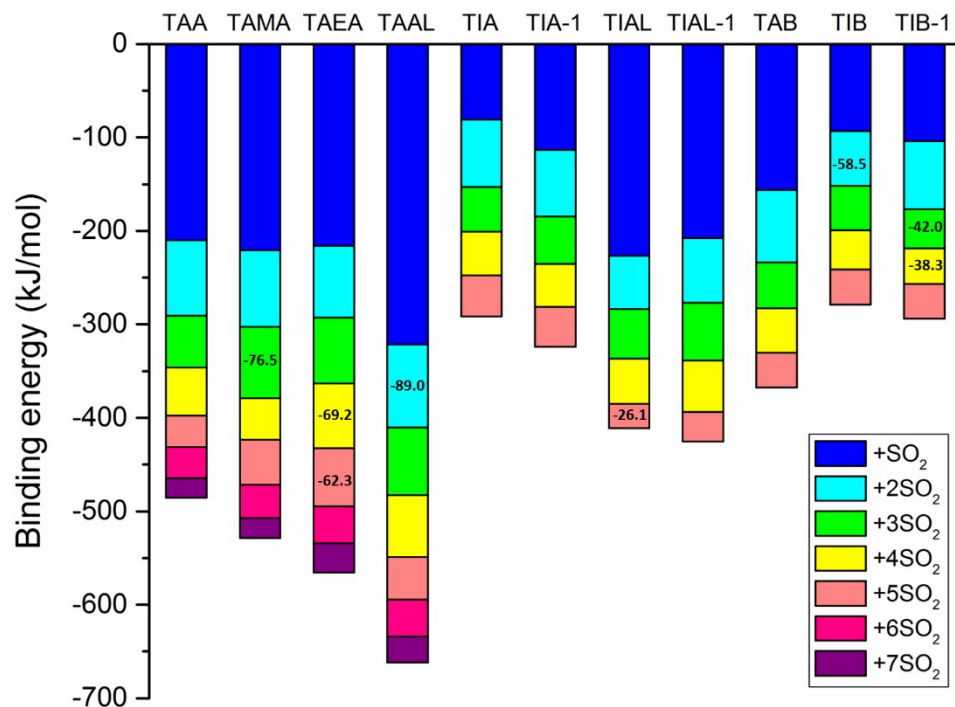


Figure S4. Stacked column plot of calculated sequential SO_2 binding energies (kJ mol^{-1}) of the studied anions. The minimum and the maximum of each binding are labeled by numbers in black during the second to the fifth SO_2 attachment.

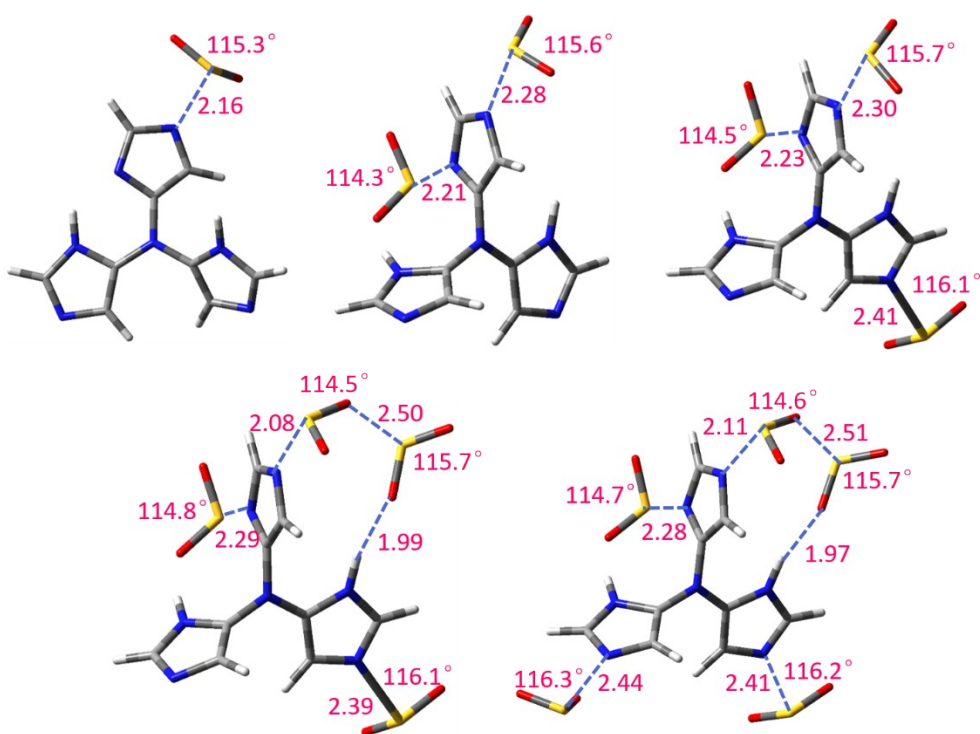
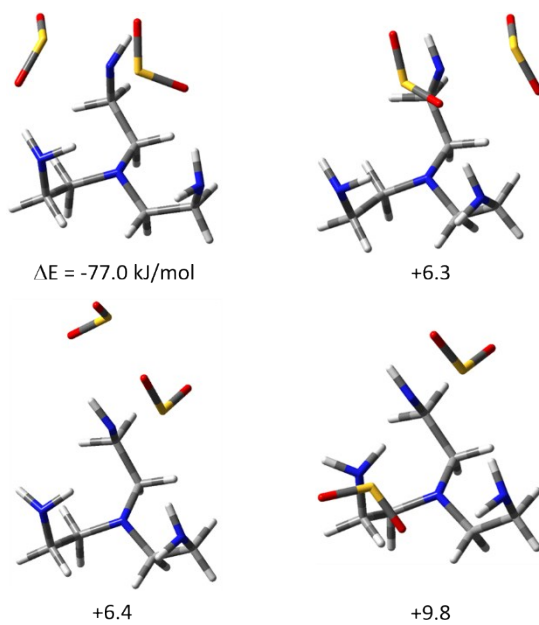


Figure S5. Configurations of the sequential SO₂ absorptions using **TIA**. The distances between N-S (Å) and the angles of ∠OSO are given.



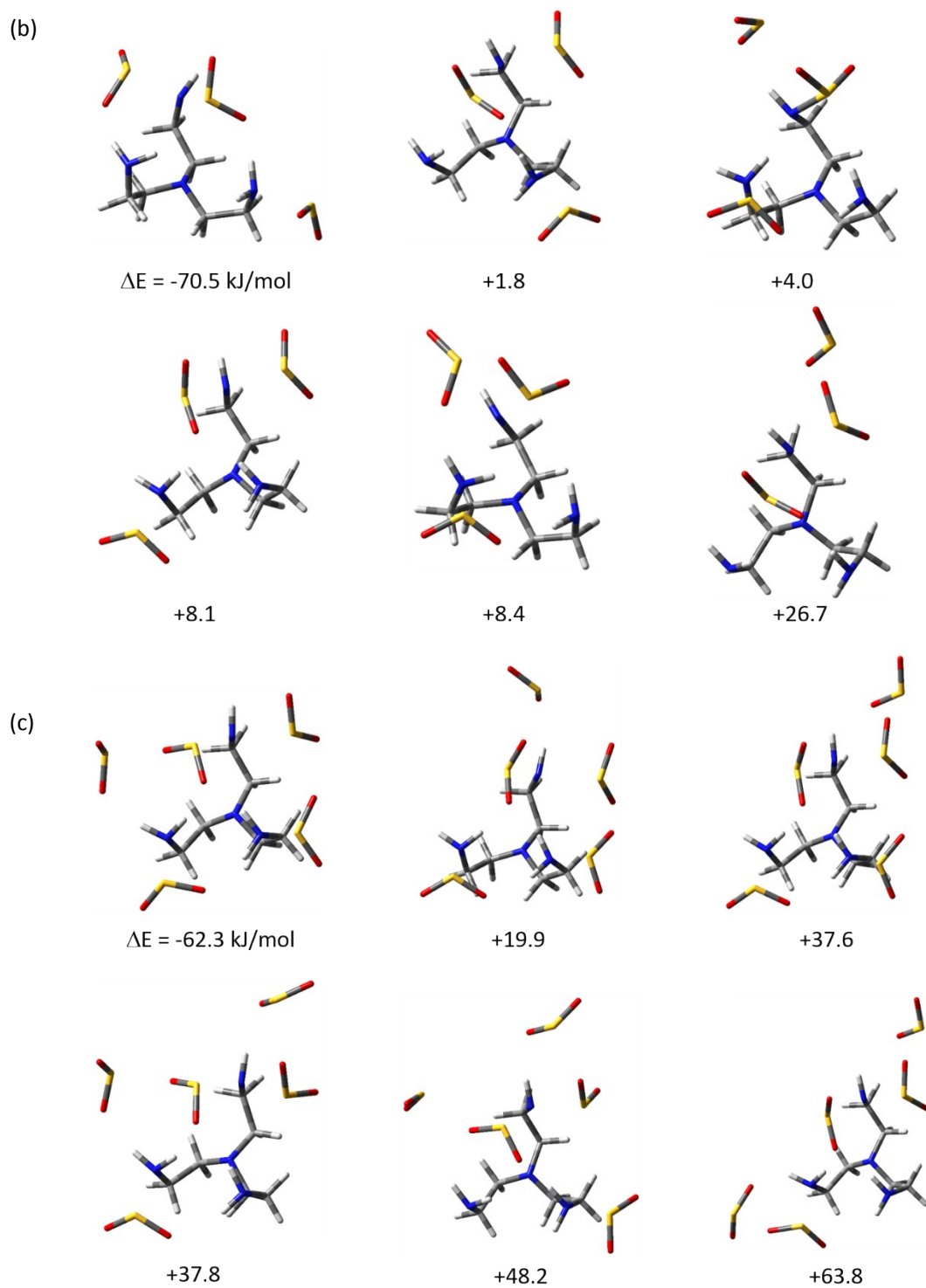


Figure S6. Various stable configurations of (a) TAEA-2SO₂, (b)TAEA-3SO₂ and (c)TAEA-5SO₂ complexes. The binding energy or the relative binding energy with respect to the most stable one (in kJ mol⁻¹) are given below each configuration.

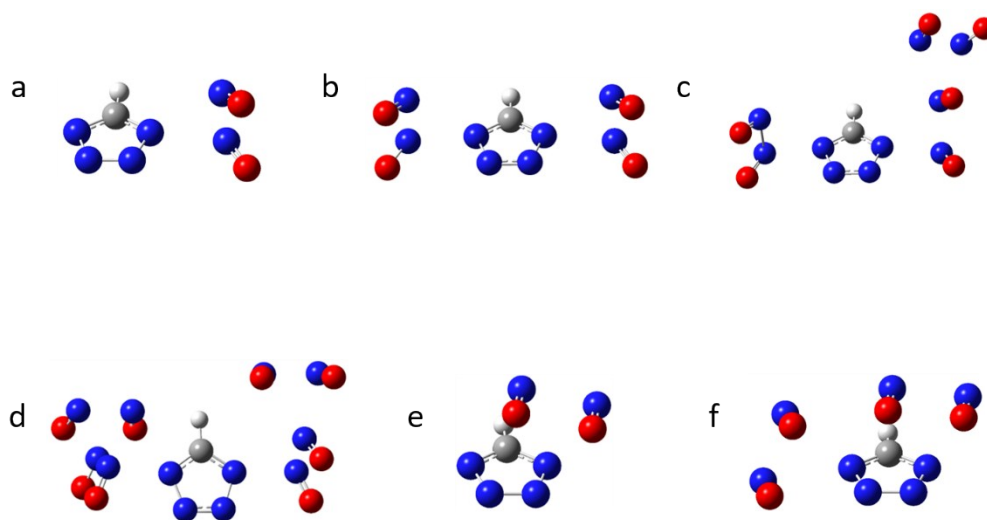


Figure S9. Multiple-site interactions in the optimized structures based on **Tetz** and NO dimers at (a-d) B3LYP/6-311++G(d,p) level and (e-f) MP2/6-31+G(d) level. (a) **Tetz**-NONO, $\Delta E = -42.9$ kJ mol⁻¹; (b) **Tetz**-2NONO, $\Delta E = -34.2$ kJ mol⁻¹; (c) **Tetz**-3NONO, $\Delta E = -26.5$ kJ mol⁻¹; (d) **Tetz**-4NONO, $\Delta E = -23.4$ kJ mol⁻¹; (e) **Tetz**-NONO, $\Delta E = -47.4$ kJ mol⁻¹; (f) **Tetz**-2NONO, $\Delta E = -45.5$ kJ mol⁻¹.

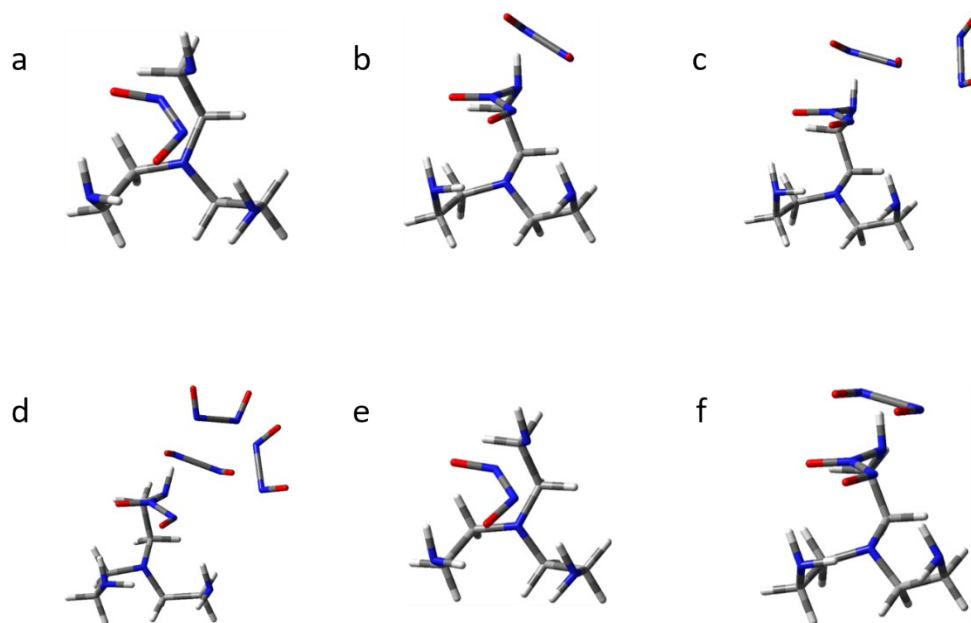


Figure S10. Multiple-site interactions in the optimized structures based on **TAEA** and NO dimer at (a-d) B3LYP/6-311++G(d,p) level and (e-f) MP2/6-31+G(d) level. (a) **TAEA**-NONO, $\Delta E = -219.0$ kJ mol⁻¹; (b) **TAEA**-2NONO, $\Delta E = -43.5$ kJ mol⁻¹; (c) **TAEA**-3NONO, $\Delta E = -31.8$ kJ mol⁻¹; (d) **TAEA**-4NONO, $\Delta E = -34.9$ kJ mol⁻¹; (e) **TAEA**-NONO, $\Delta E = -226.2$ kJ mol⁻¹; (f) **TAEA**-2NONO, $\Delta E = -69.9$ kJ mol⁻¹.

Reference

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