

Supporting Information

Anion- π interactions in $[\text{S}_4\text{N}_3]^+$ rings

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Cartesian Coordinates (BP86-D3/def2-TZVPD).

1.

S	-1.4285345	-0.2627171	-1.0677448
S	-1.4285345	-0.2627171	1.0677448
S	1.6023868	-0.2212789	1.4431941
S	1.6023868	-0.2212789	-1.4431941
N	2.2041062	-0.5882923	0.0000000
N	0.0640053	-0.3456897	-1.6823891
N	0.0640053	-0.3456897	1.6823891
Cl	-3.9144041	-0.1783653	0.0000000
Cl	1.2345828	2.4260290	0.0000000

2a.

N	0.3508939	-0.7471323	1.6836297
S	1.8454845	-1.1498014	1.4603161
S	1.8454845	-1.1498014	-1.4603161
N	2.3515883	-1.5364887	0.0000000
S	-1.0436222	-0.2766886	-1.0551491
N	-4.0334638	-0.4518182	0.0000000
O	-3.6934844	-1.6543532	0.0000000
O	-3.0868571	0.4745981	0.0000000
O	-5.2102364	-0.0664178	0.0000000
S	-1.0436222	-0.2766886	1.0551491
N	0.3508939	-0.7471323	-1.6836297
N	2.8551332	1.9056171	0.0000000
O	3.8649038	1.1450951	0.0000000
O	2.9694308	3.1520651	0.0000000
O	1.6774733	1.3789469	0.0000000

2b.

N	0.4188330	-0.7462111	1.6729280
S	1.9439106	-0.9603357	1.4656830
S	1.9439106	-0.9603357	-1.4656830
N	2.5010751	-1.2660767	0.0000000
S	-1.0402103	-0.4322064	-1.0652770
N	-4.0173973	-0.8696577	0.0000000
O	-3.5923329	-2.0435274	0.0000000
O	-3.1420719	0.1243424	0.0000000
O	-5.2202331	-0.5699054	0.0000000
S	-1.0402103	-0.4322064	1.0652770
N	0.4188330	-0.7462111	-1.6729280

N	2.7091883	2.2328362	0.0000000
O	2.5360553	1.6176816	1.1041412
O	2.5360553	1.6176816	-1.1041412
O	3.0445947	3.4341318	0.0000000

2c.

N	0.6454183	-0.7235075	1.6665269
S	2.0466527	-1.3763374	1.4791910
S	2.0315995	-1.4284600	-1.4500090
N	2.5189776	-1.8365027	0.0201484
S	-0.7291536	-0.1673848	-1.0531159
N	-3.7155767	-0.2024504	0.0176083
O	-3.4256917	-1.4184389	0.0154907
O	-2.7356856	0.6862588	0.0036676
O	-4.8776322	0.2283278	0.0319681
S	-0.7180186	-0.1285680	1.0657169
N	0.6284478	-0.7816726	-1.6457782
N	2.0760600	1.8019506	-0.0378707
O	1.6255296	2.2327315	1.0537027
O	3.0299326	0.9438002	-0.0255163
O	1.5991403	2.1702534	-1.1417302

CCDC Codes [S₄N₃]⁺:

GIRWIN
RAZQEO
SOWPID
SOWPOJ
SOWPUP
TUZLOP