Electronic Supporting Information

Noncovalent Interactions of Aromatic Heterocycle: Rotational Spectroscopy and Theoretical Calculations of the Thiazole-CF_4 and Thiazole-SF_6 Complexes

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Fig. S1 The potential energy curve of the internal rotation of -CF_3 top around C7-F9 calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory.

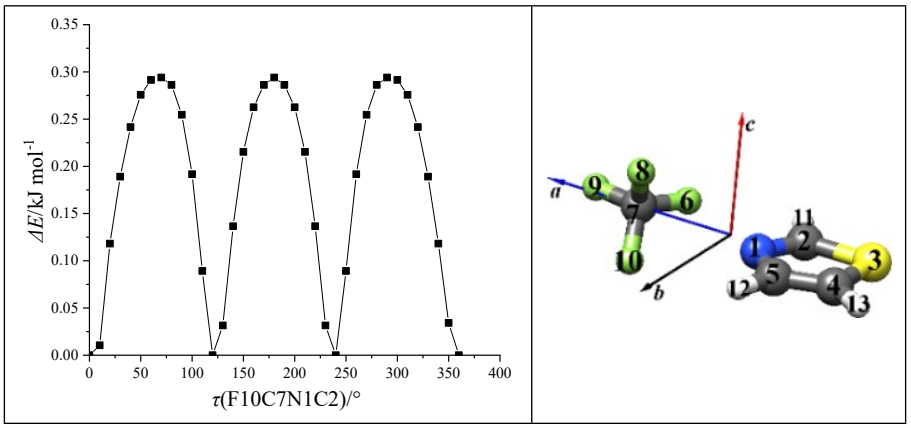

Fig. S2 Conformational interconversion pathways between low energy conformers of thiazole-CF_4 calculated at the B3LYP-D3(BJ)/def2-TZVP level.

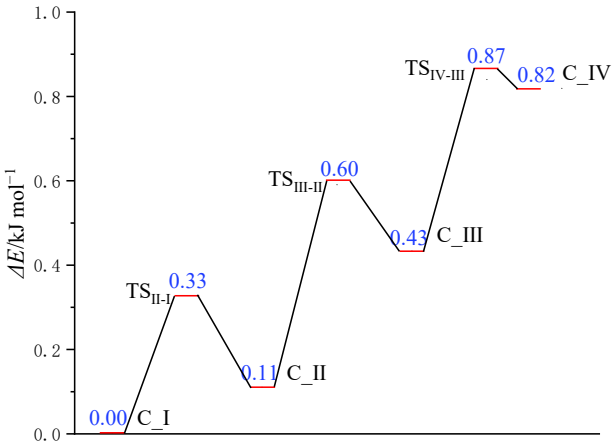

Fig. S3 Conformational interconversion pathways between low energy conformers of thiazole-SF_6 calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory.

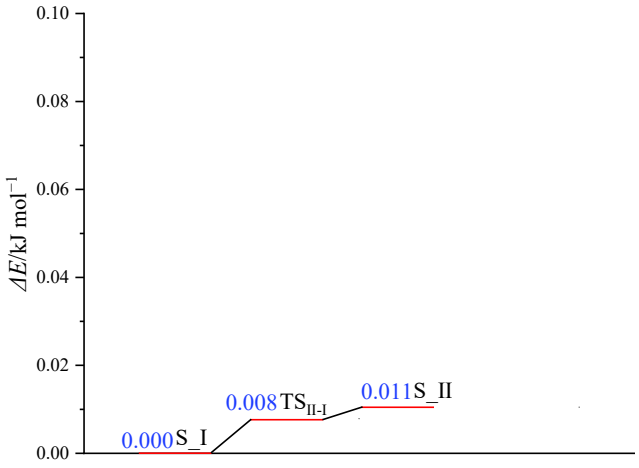

Fig. S4 Average absolute percentage deviation between experimental rotational constants and theoretical values for the thiazole-CF_4 (top) and thiazole-SF_6 (bottom) clusters calculated at different levels of theory.

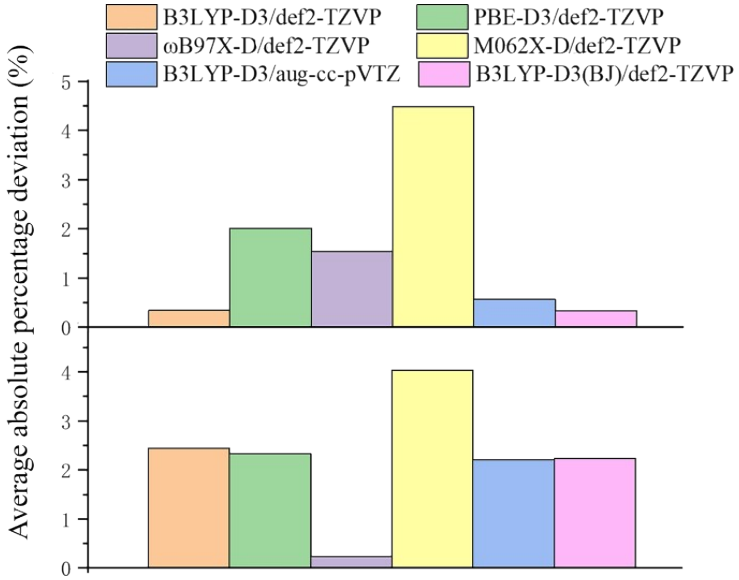

Table S1 The B3LYP-D3(BJ)/def2-TZVP calculated geometries, zero-point energies of the thiazole-SF_6 complex.

	S_I	S_II	S_III
ΔE_0/kJ mol^{-1}	0.00	0.01	1.92
A/MHz	1539	1503	1843
B/MHz	402	412	318
C/MHz	394	400	304
χ_{aa}/MHz	1.84	2.93	1.55
χ_{bb}/MHz	−1.27	−3.27	−4.44
χ_{cc}/MHz	−0.57	0.34	2.89
D_J/kHz	0.17	0.11	0.21
D_{JK}/kHz	0.78	0.92	15.61
D_K/kHz	0.14	−0.91	−9.38
d_1/Hz	−18.16	−2.49	2.77
d_2/Hz	0.91	0.40	15.18
$\lvert\mu_a\rvert$/D	0.7	0.1	0.3
$\lvert\mu_b\rvert$/D	0.9	1.3	1.6
$\lvert\mu_c\rvert$/D	1.0	0.8	0.2

Table S2 Theoretical spectroscopic parameters of thiazole-CF_4 complex calculated at different levels of theory.

	A /MHz	*B* /MHz	*C* /MHz
Exp.	3127.600	428.745	403.892
B3LYP-D3/def2-TZVP[a]	3113 (0.47%)	430(0.29%)	405(0.27%)
PBE-D3/def2-TZVP[a]	3071(1.81%)	420(2.04%)	395(2.20%)
ωB97X-D/def2-TZVP[a]	3142(0.46%)	438(2.16%)	412(2.01%)
M062X-D/def2-TZVP[a]	3163(1.13%)	456(6.36%)	428(5.97%)
B3LYP-D3/aug-cc-pVTZ[a]	3102(0.82%)	427(0.41%)	402(0.47%)
B3LYP-D3(BJ)/def2-TZVP[b]	3114(0.43%)	430(0.29%)	405(0.27%)

[a] Calculations performed using BDF program.

[b] Calculations performed using Gaussian 16.

Table S3 Theoretical spectroscopic parameters of thiazole-SF_6 complex calculated at different levels of theory.

	A /MHz	*B* /MHz	*C* /MHz
Exp.	1567.353	392.245	384.819
B3LYP-D3/def2-TZVP[a]	1537(1.94%)	403(2.74%)	395(2.65%)
PBE-D3/def2-TZVP[a]	1514(3.40%)	385(1.85%)	378(1.77%)
ωB97X-D/def2-TZVP[a]	1570(0.16%)	391(0.32%)	384(0.21%)
M062X-D/def2-TZVP[a]	1592(1.57%)	413(5.29%)	405(5.24%)
B3LYP-D3/aug-cc-pVTZ[a]	1524(2.77%)	400(1.98%)	392(1.87%)
B3LYP-D3(BJ)/def2-TZVP[b]	1539(1.81%)	402(2.49%)	394(2.39%)

[a] Calculations performed using BDF program.

[b] Calculations performed using Gaussian 16.

Table S4 Experimental transition frequencies of the thiazole-CF_4 complex.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	Sy	ν_{obs}/MHz	$\Delta\nu_{obs-}$
9	0	9	8	8	0	8	7	A	7474.5837	0.0116
9	0	9	9	8	0	8	8	A	7474.5837	0.0092
9	0	9	10	8	0	8	9	A	7474.5989	0.0060
9	0	9	8	8	0	8	7	E	7473.6756	0.0148
9	0	9	9	8	0	8	8	E	7473.6756	0.0126
9	0	9	10	8	0	8	9	E	7473.6756	-0.0060
9	1	8	9	8	1	7	8	A	7597.2697	0.0080
9	1	8	8	8	1	7	7	A	7597.2860	0.0171
9	1	8	10	8	1	7	9	A	7597.2860	0.0018
9	1	8	9	8	1	7	8	E	7595.4525	0.0001
9	1	8	8	8	1	7	7	E	7595.4525	-0.0059
9	1	8	10	8	1	7	9	E	7595.4685	-0.0054
9	1	9	9	8	1	8	8	A	7380.0877	0.0001
9	1	9	8	8	1	8	7	A	7380.0877	-0.0025
9	1	9	10	8	1	8	9	A	7380.1096	-0.0030
9	1	9	9	8	1	8	8	E	7381.2602	-0.0015
9	1	9	8	8	1	8	7	E	7381.2602	-0.0054
9	1	9	10	8	1	8	9	E	7381.2743	-0.0135
10	1	9	10	9	1	8	9	A	8439.9113	0.0075
10	1	9	9	9	1	8	8	A	8439.9113	0.0019
10	1	9	11	9	1	8	10	A	8439.9319	0.0098
10	1	9	10	9	1	8	9	E	8438.3010	-0.0002
10	1	9	9	9	1	8	8	E	8438.3010	-0.0051
10	1	9	11	9	1	8	10	E	8438.3194	0.0006
10	1	10	10	9	1	9	9	A	8198.7989	0.0018
10	1	10	9	9	1	9	8	A	8198.7989	0.0000
10	1	10	11	9	1	9	10	A	8198.8226	0.0054
10	1	10	10	9	1	9	9	E	8199.6634	-0.0007
10	1	10	9	9	1	9	8	E	8199.6634	-0.0033
10	1	10	11	9	1	9	10	E	8199.6634	-0.0215
10	3	7	10	9	3	6	9	A	8328.4326	-0.0086
10	3	7	9	9	3	6	8	A	8328.5170	-0.0108
10	3	7	11	9	3	6	10	A	8328.5170	-0.0142
10	3	8	10	9	3	7	9	A	8327.9160	0.0081
10	3	8	9	9	3	7	8	A	8327.9971	0.0021
10	3	8	11	9	3	7	10	A	8327.9971	-0.0012
10	3	8	10	9	3	7	9	E	8328.8824	-0.0636

10	3	8	9	9	3	7	8	E	8328.9912	-0.0416
10	3	8	11	9	3	7	10	E	8328.9912	-0.0450
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11	0	11	10	10	0	10	9	A	9123.9743	0.0023
11	0	11	12	10	0	10	11	A	9123.9933	0.0077
11	0	11	11	10	0	10	10	E	9122.7092	0.0111
11	0	11	10	10	0	10	9	E	9122.7092	0.0065
11	0	11	12	10	0	10	11	E	9122.7283	0.0121
11	1	10	11	10	1	9	10	A	9282.0505	0.0063
11	1	10	10	10	1	9	9	A	9282.0505	0.0015
11	1	10	12	10	1	9	11	A	9282.0675	0.0079
11	1	10	11	10	1	9	10	E	9280.5433	-0.0019
11	1	10	10	10	1	9	9	E	9280.5433	-0.0063
11	1	10	12	10	1	9	11	E	9280.5605	0.0003
11	1	11	11	10	1	10	10	A	9017.1185	-0.0004
11	1	11	10	10	1	10	9	A	9017.1185	-0.0018
11	1	11	12	10	1	10	11	A	9017.1375	0.0019
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11	2	9	10	10	2	8	9	A	9186.5322	-0.0137
11	2	9	12	10	2	8	11	A	9186.5470	-0.0093
11	2	9	11	10	2	8	10	E	9180.7672	-0.0176
11	2	9	10	10	2	8	9	E	9180.7790	-0.0166
11	2	9	12	10	2	8	11	E	9180.7926	-0.0138
11	2	10	11	10	2	9	10	A	9151.9099	0.0038
11	2	10	10	10	2	9	9	A	9151.9237	-0.0089
11	2	10	12	10	2	9	11	A	9151.9397	-0.0028
11	2	10	11	10	2	9	10	E	9159.0067	0.0205
11	2	10	10	10	2	9	9	E	9159.0282	0.0127
11	2	10	12	10	2	9	11	E	9159.0401	0.0151
11	3	8	11	10	3	7	10	A	9162.0491	0.0074
11	3	8	10	10	3	7	9	A	9162.1125	0.0078
11	3	8	12	10	3	7	11	A	9162.1125	0.0030
11	3	9	11	10	3	8	10	A	9161.1867	0.0109
11	3	9	10	10	3	8	9	A	9161.2432	0.0037
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12	0	12	11	11	0	11	10	E	9944.8224	0.0036
12	0	12	13	11	0	11	12	E	9944.8398	0.0097
12	1	11	12	11	1	10	11	A	10123.6230	0.0034
12	1	11	11	11	1	10	10	A	10123.6230	-0.0011
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12	1	11	12	11	1	10	11	E	10122.1516	-0.0057
12	1	11	11	11	1	10	10	E	10122.1516	-0.0099
12	1	11	13	11	1	10	12	E	10122.1683	-0.0022
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12	2	10	13	11	2	9	12	A	10027.2054	-0.0057
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12	2	10	11	11	2	9	10	E	10022.6041	-0.0105
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12	2	11	13	11	2	10	12	A	9982.4930	0.0006
12	2	11	12	11	2	10	11	E	9988.5868	0.0103
12	2	11	11	11	2	10	10	E	9988.6033	0.0032
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13	2	11	13	12	2	10	12	E	10865.9262	0.0057
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13	2	12	14	12	2	11	13	E	10817.6105	-0.0003
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14	0	14	13	13	0	13	12	A	11585.8116	0.0076
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14	1	13	15	13	1	12	14	A	11804.8130	-0.0007
14	1	13	14	13	1	12	13	E	11803.2795	-0.0085
14	1	13	13	13	1	12	12	E	11803.2795	-0.0131
14	1	13	15	13	1	12	14	E	11803.2919	-0.0073
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14	2	12	13	13	2	11	12	E	11710.4252	0.0192
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14	2	13	14	13	2	12	13	E	11646.2798	-0.0073
14	2	13	13	13	2	12	12	E	11646.3063	0.0038
14	2	13	15	13	2	12	14	E	11646.3063	-0.0029
15	0	15	15	14	0	14	14	A	12402.9270	-0.0057
15	0	15	14	14	0	14	13	A	12402.9457	0.0017
15	0	15	16	14	0	14	15	A	12402.9457	-0.0053
15	0	15	15	14	0	14	14	E	12400.8019	0.0047
15	0	15	14	14	0	14	13	E	12400.8216	0.0130
15	0	15	16	14	0	14	15	E	12400.8216	0.0059
15	1	14	15	14	1	13	14	A	12644.2625	0.0000
15	1	14	14	14	1	13	13	A	12644.2625	-0.0050
15	1	14	16	14	1	13	15	A	12644.2625	-0.0108
15	1	14	15	14	1	13	14	E	12642.6695	-0.0101
15	1	14	14	14	1	13	13	E	12642.6836	-0.0010
15	1	14	16	14	1	13	15	E	12642.6836	-0.0067
15	1	15	15	14	1	14	14	A	12286.0497	0.0037
15	1	15	14	14	1	14	13	A	12286.0497	0.0018
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15	1	15	14	14	1	14	13	E	12286.2379	-0.0095
15	1	15	16	14	1	14	15	E	12286.2379	-0.0178
15	2	13	14	14	2	12	13	A	12556.7760	-0.0067
15	2	13	16	14	2	12	15	A	12556.7892	-0.0001
15	2	13	15	14	2	12	14	A	12556.7892	0.0024
15	2	13	14	14	2	12	13	E	12555.9583	0.0349
15	2	13	16	14	2	12	15	E	12555.9583	0.0282
15	2	13	15	14	2	12	14	E	12555.9583	0.0293

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15	2	14	16	14	2	13	15	A	12471.7902	0.0127
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15	2	14	16	14	2	13	15	E	12474.7814	-0.0111
16	0	16	16	15	0	15	15	A	13218.3335	-0.0139
16	0	16	15	15	0	15	14	A	13218.3526	-0.0069
16	0	16	17	15	0	15	16	A	13218.3606	-0.0051
16	0	16	16	15	0	15	15	E	13215.9879	-0.0008
16	0	16	15	15	0	15	14	E	13216.0090	0.0081
16	0	16	17	15	0	15	16	E	13216.0090	0.0019
16	1	15	16	15	1	14	15	A	13482.8608	-0.0019
16	1	15	15	15	1	14	14	A	13482.8608	-0.0072
16	1	15	17	15	1	14	16	A	13482.8608	-0.0123
16	1	15	16	15	1	14	15	E	13481.1857	-0.0048
16	1	15	15	15	1	14	14	E	13481.1857	-0.0101
16	1	15	17	15	1	14	16	E	13481.1857	-0.0152
16	1	16	16	15	1	15	15	A	13102.1011	0.0057
16	1	16	15	15	1	15	14	A	13102.1011	0.0035
16	1	16	17	15	1	15	16	A	13102.1011	-0.0038
16	1	16	16	15	1	15	15	E	13102.2151	-0.0072
16	1	16	15	15	1	15	14	E	13102.2151	-0.0094
16	1	16	17	15	1	15	16	E	13102.2268	-0.0050

Table S5 Experimental transition frequencies of the thiazole-SF_6 complex.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$ /MHz
4	3	1	4	3	2	2	3	9002.1879	0.0017
4	3	1	5	3	2	2	4	9002.3692	-0.0008
4	3	1	3	3	2	2	2	9002.4174	0.0001
4	3	1	4	3	2	1	3	9002.0094	-0.0001
4	3	1	5	3	2	1	4	9002.1879	-0.0071
4	3	1	3	3	2	1	2	9002.2445	0.0016
4	3	2	4	3	2	1	3	9002.0094	0.0005
4	3	2	5	3	2	1	4	9002.1879	-0.0064
4	3	2	3	3	2	1	2	9002.2445	0.0024
4	3	2	4	3	2	2	3	9002.1879	0.0024
4	3	2	5	3	2	2	4	9002.3692	-0.0001
4	3	2	3	3	2	2	2	9002.4174	0.0008
4	4	0	4	3	3	1	3	11359.7890	0.0023
4	4	0	3	3	3	1	2	11359.8480	0.0033
4	4	0	5	3	3	1	4	11359.8750	-0.0053
4	4	1	4	3	3	0	3	11359.7890	0.0024
4	4	1	3	3	3	0	2	11359.8480	0.0034
4	4	1	5	3	3	0	4	11359.8750	-0.0052
5	3	2	5	4	2	3	4	9779.3319	0.0033
5	3	2	6	4	2	3	5	9779.4870	0.0020
5	3	2	4	4	2	3	3	9779.5220	-0.0059
5	3	2	5	4	2	2	4	9778.7984	-0.0019
5	3	2	6	4	2	2	5	9778.9585	-0.0009
5	3	2	4	4	2	2	3	9779.0018	-0.0014
5	3	3	5	4	2	2	4	9778.7984	0.0009
5	3	3	6	4	2	2	5	9778.9585	0.0019
5	3	3	4	4	2	2	3	9779.0018	0.0014
5	3	3	5	4	2	3	4	9779.3319	0.0062
5	3	3	6	4	2	3	5	9779.4870	0.0049
5	3	3	4	4	2	3	3	9779.5220	-0.0030
5	4	1	5	4	3	2	4	12136.7015	-0.0052
5	4	1	6	4	3	2	5	12136.8378	-0.0056
5	4	1	4	4	3	2	3	12136.8751	0.0137
5	4	1	5	4	3	1	4	12136.7015	-0.0044
5	4	1	6	4	3	1	5	12136.8378	-0.0048
5	4	1	4	4	3	1	3	12136.8751	0.0144
5	4	2	5	4	3	1	4	12136.7015	-0.0044

5	4	2	6	4	3	1	5	12136.8378	-0.0048
5	4	2	4	4	3	1	3	12136.8751	0.0144
5	4	2	5	4	3	2	4	12136.7015	-0.0052
5	4	2	6	4	3	2	5	12136.8378	-0.0055
5	4	2	4	4	3	2	3	12136.8751	0.0137
5	5	0	5	4	4	1	4	14494.3498	-0.0016
5	5	0	4	4	4	1	3	14494.3844	-0.0056
5	5	0	6	4	4	1	5	14494.4130	-0.0032
5	5	0	5	4	4	0	4	14494.3498	-0.0016
5	5	0	4	4	4	0	3	14494.3844	-0.0056
5	5	0	6	4	4	0	5	14494.4130	-0.0032
5	5	1	5	4	4	0	4	14494.3498	-0.0016
5	5	1	4	4	4	0	3	14494.3844	-0.0056
5	5	1	6	4	4	0	5	14494.4130	-0.0032
5	5	1	5	4	4	1	4	14494.3498	-0.0016
5	5	1	4	4	4	1	3	14494.3844	-0.0056
5	5	1	6	4	4	1	5	14494.4130	-0.0032
6	5	1	6	5	4	2	5	15271.2105	-0.0061
6	5	1	7	5	4	2	6	15271.3230	0.0022
6	5	1	5	5	4	2	4	15271.3230	-0.0041
6	5	1	6	5	4	1	5	15271.2105	-0.0061
6	5	1	7	5	4	1	6	15271.3230	0.0022
6	5	1	5	5	4	1	4	15271.3230	-0.0040
6	5	2	6	5	4	1	5	15271.2105	-0.0061
6	5	2	7	5	4	1	6	15271.3230	0.0022
6	5	2	5	5	4	1	4	15271.3230	-0.0040
6	5	2	6	5	4	2	5	15271.2105	-0.0061
6	5	2	7	5	4	2	6	15271.3230	0.0022
6	5	2	5	5	4	2	4	15271.3230	-0.0041
6	6	0	6	5	5	1	5	17628.8328	0.0058
6	6	0	5	5	5	1	4	17628.8729	0.0183
6	6	0	7	5	5	1	6	17628.8729	-0.0016
6	6	0	6	5	5	0	5	17628.8328	0.0058
6	6	0	5	5	5	0	4	17628.8729	0.0183
6	6	0	7	5	5	0	6	17628.8729	-0.0016
6	6	1	6	5	5	0	5	17628.8328	0.0058
6	6	1	5	5	5	0	4	17628.8729	0.0183
6	6	1	7	5	5	0	6	17628.8729	-0.0016
6	6	1	6	5	5	1	5	17628.8328	0.0058
6	6	1	5	5	5	1	4	17628.8729	0.0183
6	6	1	7	5	5	1	6	17628.8729	-0.0016

7	5	2	7	6	4	3	6	16048.0660	-0.0001
7	5	2	8	6	4	3	7	16048.1721	-0.0018
7	5	2	6	6	4	3	5	16048.1956	0.0079
7	5	2	7	6	4	2	6	16048.0660	0.0000
7	5	2	8	6	4	2	7	16048.1721	-0.0018
7	5	2	6	6	4	2	5	16048.1956	0.0079
7	5	3	7	6	4	2	6	16048.0660	0.0000
7	5	3	8	6	4	2	7	16048.1721	-0.0018
7	5	3	6	6	4	2	5	16048.1956	0.0079
7	5	3	7	6	4	3	6	16048.0660	-0.0001
7	5	3	8	6	4	3	7	16048.1721	-0.0018
7	5	3	6	6	4	3	5	16048.1956	0.0079
7	6	1	7	6	5	2	6	18405.6238	0.0010
7	6	1	8	6	5	2	7	18405.6988	-0.0055
7	6	1	6	6	5	2	5	18405.6988	-0.0068
7	6	1	7	6	5	1	6	18405.6238	0.0010
7	6	1	8	6	5	1	7	18405.6988	-0.0055
7	6	1	6	6	5	1	5	18405.6988	-0.0068
7	6	2	7	6	5	1	6	18405.6238	0.0010
7	6	2	8	6	5	1	7	18405.6988	-0.0055
7	6	2	6	6	5	1	5	18405.6988	-0.0068
7	6	2	7	6	5	2	6	18405.6238	0.0010
7	6	2	8	6	5	2	7	18405.6988	-0.0055
7	6	2	6	6	5	2	5	18405.6988	-0.0068
8	2	6	7	7	1	7	6	9863.7161	0.0025
8	2	6	9	7	1	7	8	9863.7161	0.0030
8	2	6	8	7	1	7	7	9863.7742	0.0055
8	2	6	8	7	1	6	7	9655.7555	0.0010
8	2	6	9	7	1	6	8	9655.9080	0.0043
8	2	6	7	7	1	6	6	9655.9315	-0.0022
8	2	7	8	7	1	6	7	9648.3908	-0.0013
8	2	7	9	7	1	6	8	9648.5542	0.0013
8	2	7	7	7	1	6	6	9648.5865	0.0021
8	2	7	7	7	1	7	6	9856.3620	-0.0021
8	2	7	9	7	1	7	8	9856.3620	-0.0001
8	2	7	8	7	1	7	7	9856.4128	0.0064
8	5	3	8	7	4	4	7	16824.8694	-0.0019
8	5	3	9	7	4	4	8	16824.9654	-0.0069
8	5	3	7	7	4	4	6	16824.9906	0.0041
8	5	4	8	7	4	3	7	16824.8694	-0.0019
8	5	4	9	7	4	3	8	16824.9654	-0.0068

8	5	4	7	7	4	3	6	16824.9906	0.0041
8	6	2	8	7	5	3	7	19182.3871	-0.0018
8	6	2	9	7	5	3	8	19182.4787	0.0002
8	6	2	7	7	5	3	6	19182.4787	-0.0076
8	6	3	8	7	5	2	7	19182.3871	-0.0018
8	6	3	9	7	5	2	8	19182.4787	0.0002
8	6	3	7	7	5	2	6	19182.4787	-0.0076
9	1	8	8	8	0	8	7	8343.3994	0.0048
9	1	8	10	8	0	8	9	8343.3994	0.0017
9	1	8	9	8	0	8	8	8343.4801	-0.0137
9	2	7	8	8	1	8	7	10674.5129	0.0047
9	2	7	10	8	1	8	9	10674.5129	0.0028
9	2	7	9	8	1	8	8	10674.5847	0.0043
9	2	7	9	8	1	7	8	10407.2141	0.0033
9	2	7	10	8	1	7	9	10407.3505	0.0039
9	2	8	9	8	1	7	8	10395.6526	-0.0019
9	2	8	10	8	1	7	9	10395.8034	-0.0014
9	2	8	8	8	1	7	7	10395.8272	-0.0032
9	2	8	8	8	1	8	7	10662.9620	-0.0060
9	2	8	10	8	1	8	9	10662.9620	-0.0063
9	2	8	9	8	1	8	8	10663.0235	-0.0007
10	0	10	10	9	0	9	9	7764.1472	0.0006
10	0	10	11	9	0	9	10	7764.1472	-0.0003
10	0	10	9	9	0	9	8	7764.1472	-0.0064
10	1	9	9	9	0	9	8	9160.0964	0.0024
10	1	9	11	9	0	9	10	9160.0964	-0.0016
10	1	9	10	9	0	9	9	9160.1918	-0.0077
10	1	9	11	9	1	8	10	7805.5482	0.0058
10	1	9	10	9	1	8	9	7805.5482	0.0006
10	1	9	9	9	1	8	8	7805.5482	-0.0007
10	1	10	10	9	0	9	9	8751.9550	-0.0016
10	1	10	11	9	0	9	10	8752.0725	0.0094
10	1	10	9	9	0	9	8	8752.0725	-0.0073
10	1	10	11	9	1	9	10	7731.4116	-0.0063
10	1	10	10	9	1	9	9	7731.4116	-0.0107
10	1	10	9	9	1	9	8	7731.4116	-0.0106
10	2	9	11	9	2	8	10	7768.9444	-0.0030
10	2	9	9	9	2	8	8	7768.9444	-0.0069
10	2	9	10	9	2	8	9	7768.9650	0.0025
10	3	7	11	9	3	6	10	7770.5810	0.0000
10	3	7	9	9	3	6	8	7770.5810	-0.0011

10	3	7	10	9	3	6	9	7770.6133	-0.0001
10	3	8	11	9	3	7	10	7770.5060	0.0067
10	3	8	9	9	3	7	8	7770.5060	0.0056
10	3	8	10	9	3	7	9	7770.5353	0.0037
11	0	11	11	10	0	10	10	8539.0719	0.0010
11	0	11	12	10	0	10	11	8539.0719	-0.0006
11	0	11	10	10	0	10	9	8539.0719	-0.0057
11	1	10	10	10	0	10	9	9981.5086	-0.0009
11	1	10	12	10	0	10	11	9981.5086	-0.0056
11	1	10	11	10	0	10	10	9981.6263	0.0057
11	1	10	12	10	1	9	11	8585.5673	0.0035
11	1	10	11	10	1	9	10	8585.5673	-0.0003
11	1	10	10	10	1	9	9	8585.5673	-0.0019
11	1	11	11	10	0	10	10	9491.8962	0.0006
11	1	11	12	10	0	10	11	9492.0018	0.0039
11	1	11	10	10	0	10	9	9492.0018	-0.0102
11	1	11	12	10	1	10	11	8504.0826	0.0003
11	1	11	11	10	1	10	10	8504.0826	-0.0028
11	1	11	10	10	1	10	9	8504.0826	-0.0032
11	2	10	12	10	2	9	11	8545.4492	-0.0015
11	2	10	10	10	2	9	9	8545.4492	-0.0050
11	2	10	11	10	2	9	10	8545.4642	0.0021
11	3	8	12	10	3	7	11	8547.6677	0.0037
11	3	8	10	10	3	7	9	8547.6677	0.0021
11	3	8	11	10	3	7	10	8547.6885	-0.0003
11	3	9	12	10	3	8	11	8547.5375	0.0064
11	3	9	10	10	3	8	9	8547.5375	0.0048
11	3	9	11	10	3	8	10	8547.5526	-0.0031
12	0	12	12	11	0	11	11	9313.5854	0.0018
12	0	12	13	11	0	11	12	9313.5854	-0.0003
12	0	12	11	11	0	11	10	9313.5854	-0.0046
12	1	11	13	11	1	10	12	9365.4313	0.0040
12	1	11	12	11	1	10	11	9365.4313	0.0012
12	1	11	11	11	1	10	10	9365.4313	-0.0006
12	1	12	12	11	0	11	11	10229.4420	0.0000
12	1	12	13	11	0	11	12	10229.5445	0.0043
12	1	12	11	11	0	11	10	10229.5445	-0.0080
12	1	12	13	11	1	11	12	9276.6175	0.0026
12	1	12	12	11	1	11	11	9276.6175	0.0002
12	1	12	11	11	1	11	10	9276.6175	-0.0005
12	2	10	13	11	2	9	12	9331.7510	0.0032

12	2	10	11	11	2	9	10	9331.7510	0.0002
12	2	10	12	11	2	9	11	9331.7696	0.0092
12	2	11	13	11	2	10	12	9321.8404	-0.0011
12	2	11	11	11	2	10	10	9321.8404	-0.0042
12	2	11	12	11	2	10	11	9321.8492	-0.0010
13	0	13	13	12	0	12	12	10087.6657	0.0093
13	0	13	14	12	0	12	13	10087.6657	0.0065
13	0	13	12	12	0	12	11	10087.6657	0.0029
13	1	12	14	12	1	11	13	10145.1175	0.0012
13	1	12	13	12	1	11	12	10145.1175	-0.0007
13	1	12	12	12	1	11	11	10145.1175	-0.0027
13	1	13	14	12	1	12	13	10049.0109	0.0045
13	1	13	13	12	1	12	12	10049.0109	0.0027
13	1	13	12	12	1	12	11	10049.0109	0.0018
13	2	11	14	12	2	10	13	10110.6542	-0.0078
13	2	11	12	12	2	10	11	10110.6542	-0.0104
13	2	11	13	12	2	10	12	10110.6542	-0.0188
13	2	12	14	12	2	11	13	10098.1103	0.0005
13	2	12	12	12	2	11	11	10098.1103	-0.0022
13	2	12	13	12	2	11	12	10098.1103	-0.0062
14	0	14	14	13	0	13	13	10861.2709	0.0056
14	0	14	15	13	0	13	14	10861.2709	0.0024
14	0	14	13	13	0	13	12	10861.2709	-0.0007
14	1	13	15	13	1	12	14	10924.6161	0.0026
14	1	13	14	13	1	12	13	10924.6161	0.0012
14	1	13	13	13	1	12	12	10924.6161	-0.0008
14	1	14	15	13	1	13	14	10821.2494	0.0017
14	1	14	14	13	1	13	13	10821.2494	0.0006
14	1	14	13	13	1	13	12	10821.2494	-0.0005

Table S6 The partial r_0 structure of the observed conformers together with theoretical structure (r_e).

	r_0	r_e
thiazole-CF_4		
r(N1C7)/Å	3.407(2)	3.412
∠C2N1C7/°	110.5(3)	108.9
thiazole-SF_6		
r(N1S7)/Å	4.092(7)	4.019
∠C2N1S7/°	[89.636][a]	89.636

[a] Parameter fixed at the r_e value.