Electronic Supplementary Information

Elucidating the non-covalent interactions in the thiazole-carbon dioxide complexes through rotational spectroscopy and theoretical computations

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Table S1. Geometries and spectroscopic parameters of the four most stable isomers of the thiazole-$(CO_2)_2$ complex calculated at the B3LYP-D3BJ/def2-TZVP level of theory.

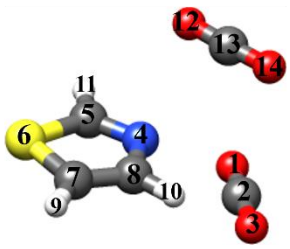
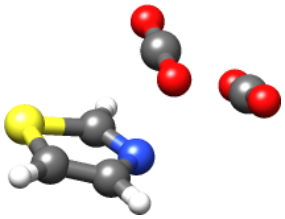
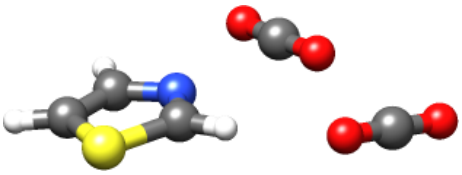
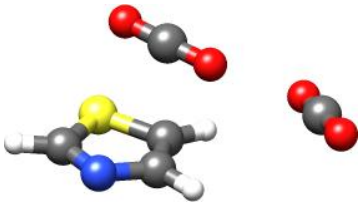
Isomer	TZ-2CO_2_1	TZ-2CO_2_2
		
ΔE (kJmol^{-1})	0	2.4
A, B, C (MHz)	1269, 593, 479	1139, 733, 547
$\lvert\mu_{a,\ b,\ c}\rvert$ (D)	2.3, 0.2, 0.2	1.9, 0.6, 0.3
Isomer	TZ-2CO_2_3	TZ-2CO_2_4
		
ΔE (kJmol^{-1})	4.9	12.0
A, B, C (MHz)	1162, 487, 345	1381, 535, 465
$\lvert\mu_{a,\ b,\ c}\rvert$ (D)	1.8, 1.0, 0.0	0.2, 0.6, 1.5

Table S2. The r_e coordinates of the most stable isomer of the thiazole-$(CO_2)_2$ complex calculated at the B3LYP-D3BJ/def2-TZVP level of theory.

Atom	*a*/Å	*b*/Å	*c*/Å
N1	−0.512	−0.075	0.110
C2	−1.235	−0.897	0.936
C3	−2.588	−0.811	0.804
S4	−2.981	0.346	−0.405
C5	−1.297	0.632	−0.647
H6	−0.945	1.354	−1.369
H7	−0.713	−1.552	1.618
H8	−3.350	−1.352	1.338
O9	2.283	−0.808	−1.348
C10	1.956	−1.566	−0.534
O11	1.656	−2.349	0.267
O12	1.415	2.385	−0.331
C13	1.865	1.666	0.460
O14	2.342	0.976	1.260

Table S3. Geometries and spectroscopic parameters of the four most stable isomers of the thiazole-$(CO_2)_3$ complex calculated at the B3LYP-D3BJ/def2-TZVP level of theory.

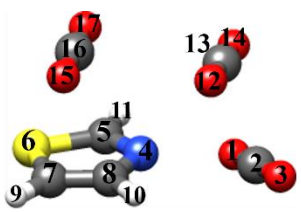
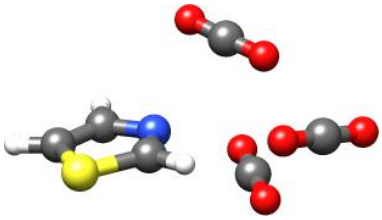
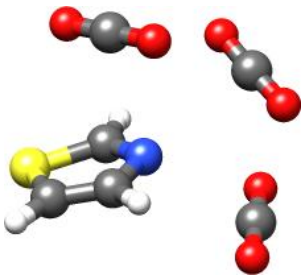
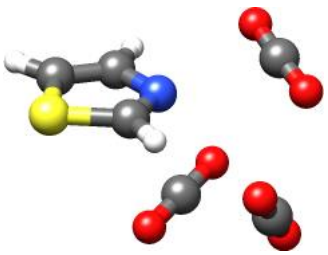
Isomer	TZ-3CO_2_1	TZ-3CO_2_2
		
ΔE (kJmol^{-1})	0	0.5
A, B, C (MHz)	711, 464, 335	705, 394, 334
$\lvert\mu_{a,\ b,\ c}\rvert$ (D)	1.8, 1.3, 0.0	2.2, 0.7, 0.1
Isomer	TZ-3CO_2_3	TZ-3CO_2_4
		
ΔE (kJmol^{-1})	0.7	2.0
A, B, C (MHz)	647, 505, 350	667, 438, 395
$\lvert\mu_{a,\ b,\ c}\rvert$ (D)	2.0, 1.3, 0.2	2.1, 0.4, 0.2

Table S4. The r_e coordinates of the most stable isomer of the thiazole-$(CO_2)_3$ complex calculated at the B3LYP-D3BJ/def2-TZVP level of theory.

Atom	*a*/Å	*b*/Å	*c*/Å
N1	−0.348	0.785	0.349
C2	0.644	0.742	1.294
C3	1.733	1.517	1.030
S4	1.512	2.339	−0.464
C5	−0.029	1.581	−0.628
H6	−0.662	1.767	−1.482
H7	0.522	0.113	2.163
H8	2.626	1.642	1.619
O9	−3.283	1.212	−0.581
C10	−3.247	0.431	0.275
O11	−3.256	−0.350	1.132
O12	−0.309	−2.382	0.557
C13	−0.972	−2.039	−0.330
O14	−1.637	−1.727	−1.227
O15	3.120	−1.688	0.753
C16	2.545	−1.457	−0.227
O17	1.984	−1.231	−1.217

Table S5. The result of NBO analysis for the most stable isomer of the thiazole-CO_2 complex.

From thiazole to CO_2			From CO_2 to thiazole		
Donor NBO[a]	Acceptor NBO[b]	$E^{(2)}$/kJmol^{-1}	Donor NBO	Acceptor NBO	$E^{(2)}$/kJmol^{-1}
BD(1)C8−N4	RY*(4)C2	0.21	BD(1)C2−O1	RY*(8)N4	0.59
BD(1)C8−N4	RY*(6)C2	0.84	BD(1)C2−O1	RY*(1)N4	0.71
BD(1)C8−N4	RY*(5)O1	0.29	BD(1)C2−O1	RY*(1)N4	0.21
BD(1)C8−H10	RY*(9)C2	0.42	BD(2)C2−O1	LP(2)N4	0.29
BD(1)C5−N4	RY*(1)C2	0.67	BD(3)C2−O1	RY*(3)N4	2.34
BD(1)C5−N4	RY*(7)C2	0.42	BD(3)C2−O1	RY*(6)N4	0.21
BD(1)C5−H11	RY*(7)C2	0.42	BD(3)C2−O1	RY*(1)N4	0.54
LP(1)N4	RY*(5)C2	0.33	BD(3)C2−O1	BD*(1)C2−N4	0.84
LP(1)N4	RY*(5)C2	0.29	BD(1)C2−O1	RY*(1)N4	0.37
LP(1)N4	RY*(24)C2	0.33	BD(3)O3	BD*(1)S6−C2	0.21
LP(1)N4	RY*(3)O1	0.67	BD(3)C2−O1	BD*(1)C8−N4	0.33
LP(1)N4	RY*(3)O3	0.29			
LP(1)N4	BD*(3)C2−O1	5.90			
LP(2)N4	BD*(2)C2−O1	0.33			

[a]BD for 2-center bond, LP for 1-center valence lone pair the unstarred and starred labels corresponding to Lewis and non-Lewis NBOs, respectively. [b]RY* for 1-center Rydberg, and BD* for 2-center antibond, the unstarred and starred labels corresponding to Lewis and non-Lewis NBOs, respectively.

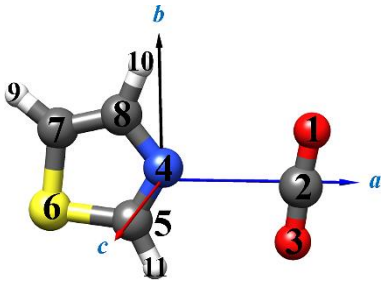


Table S6. The result of NBO analysis for the most stable isomer of thiazole-$(CO_2)_2$ complex.

From thiazole to CO_2[a]			From thiazole to CO_2[b]		
Donor NBO[c]	Acceptor NBO[d]	$E^{(2)}$/kJmol^{-1}	Donor NBO	Acceptor NBO	$E^{(2)}$/kJmol^{-1}
BD(1)C2−N1	RY*(1)C10	0.42	BD(1)C2−N1	RY*(8)C13	0.25
BD(1)C2−H7	RY*(8)C10	0.46	BD(1)C2−H7	RY*(1)C13	0.25
BD(1)C2−H7	RY*(4)O11	0.25	BD(1)C5−N1	RY*(1)C13	0.38
BD(1)C5−H6	RY*(11)C10	0.29	BD(2)C5−N1	RY*(2)C13	0.25
LP(1)N1	RY*(5)C10	0.29	BD(1)C5−H6	RY*(3)C13	0.54
LP(1)N1	RY*(3)O11	0.25	BD(1)C5−H6	RY*(6)O12	0.25
LP(1)N1	BD*(3)C10−O11	4.68	BD(1)C5−H6	RY*(1)O12	0.25
LP(2)N1	BD*(3)C10−O11	2.01	LP(1)N1	RY*(1)C13	0.29
			LP(1)N1	RY*(1)O14	0.25
			LP(1)N1	BD*(1)C13−O14	0.38
			LP(1)N1	BD*(1)C13−O14	3.55
			LP(1)N1	BD*(1)C13−O14	0.75
			LP(1)N1	BD*(1)C13−O14	0.96
From CO_2[a] to thiazole			From CO_2[a] to CO_2[b]		
BD(1)C10−O11	RY*(2)N1	0.42	LP(2)O9	BD*(2)C13−O14	0.54
BD(3)C10−O11	LP(2)N1	0.42	LP(2)O9	BD*(3)C13−O14	0.84
BD(3)C10−O11	BD*(1)C2−C3	0.33	LP(3)O9	BD*(2)C13−O14	0.25
BD(3)C10−O11	BD*(2)C2−C3	0.25			
BD(3)C10−O11	BD*(1)C5−N1	0.29			
From CO_2[b] to thiazole			From CO_2[b] to CO_2[a]		
BD(1)C13−O14	RY*(2)N1	0.21	BD(2)C13−O14	BD*(2)C10−O9	0.25
BD(3)C13−O14	LP(2)N1	0.21	BD(3)C13−O14	BD*(2)C10−O9	0.59
BD(1)C13−O12	RY*(2)N1	0.29	BD(3)C13−O14	BD*(3)C10−O9	0.25
LP(2)O12	RY*(10)N1	0.25	LP(1)O14	BD*(2)C10−O9	0.25
LP(2)O12	BD*(1)S4−C5	0.67			
LP(2)O12	BD*(2)S4−C5	0.67			

[a]The carbon atom number 10 of CO_2. [b]The carbon atom number 13 of CO_2. [c]BD for 2−center bond, LP for 1−center valence lone pair the unstarred and starred labels corresponding to Lewis and non−Lewis NBOs, respectively. [d]RY* for 1−center Rydberg, and BD* for 2−center antibond, the unstarred and starred labels corresponding to Lewis and non−Lewis NBOs, respectively.

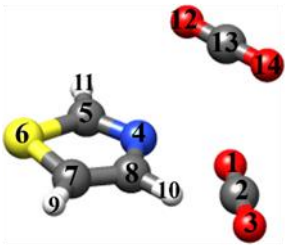


Table S7. The result of NBO analysis for the most stable isomer of the thiazole-$(CO_2)_3$ complex.

From thiazole to CO_2[a]			From thiazole to CO_2[b]		
Donor NBO[c]	Acceptor NBO[d]	$E^{(2)}$/kJmol^{-1}	Donor NBO	Acceptor NBO	$E^{(2)}$/kJmol^{-1}
BD(1)C2−N1	RY*(4)C10	0.25	BD(1)C2−N1	RY*(1)C13	0.29
BD(1)C2−N1	RY*(6)C10	0.33	BD(1)C2−H7	RY*(8)C13	0.29
BD(1)C5−N1	RY*(1)C10	0.50	BD(1)C2−H7	RY*(5)O12	0.29
BD(1)C5−N1	RY*(8)C10	0.21	LP(1)N1	RY*(4)C13	0.25
BD(1)C5−H6	RY*(8)C10	0.38	LP(1)N1	BD*(2)C13−O14	0.42
BD(1)C5−H6	RY*(5)O9	0.38	LP(1)N1	BD*(3)C13−O14	2.80
LP(1)N1	RY*(5)C10	0.21	LP(2)N1	BD*(2)C13−O14	1.38
LP(1)N1	RY*(3)O9	0.29	LP(2)N1	BD*(3)C13−O14	2.42
LP(1)N1	BD*(2)C10−O11	0.63			
LP(1)N1	BD*(3)C10−O11	4.77			
LP(2)N1	BD*(2)C10−O11	0.67			
LP(2)N1	BD*(3)C10−O11	0.50			
From thiazole to CO_2[c]			From CO_2[a] to thiazole		
BD(1)C2−C3	RY*(6)C16	0.21	BD(1)C10−O11	RY*(2)N1	0.33
BD(1)C2−C3	RY*(7)C16	0.21	BD(1)C10−O9	RY*(2)N1	0.42
BD(2)C2−C3	RY*(5)C16	0.25	LP(2)O9	RY*(10)N1	0.38
BD(2)C2−C3	BD*(2)C16−O15	2.47	LP(2)O9	BD*(1)S4−C5	0.67
			LP(2)O9	BD*(2)S4−C5	0.38
			BD(3)C10−O11	BD*(1)C2−N1	0.21
From CO_2[b] to thiazole			From CO_2[b] to CO_2[a]		
BD(1)C13−O12	RY*(2)N1	0.29	BD(3)C13−O14	BD*(2)C10−O11	0.29
BD(2)C13−O14	LP(2)N1	0.25	BD(3)C13−O14	BD*(3)C10−O11	0.38
BD(3)C13−O14	LP(2)N1	0.42	LP(1)O14	BD*(2)C10−O11	0.25
LP(2)O12	BD*(2)C2−C3	0.79			
From CO_2[b] to CO_2[c]			From CO_2[c] to thiazole		
LP(1)O12	BD*(3)C16−O15	0.46	BD(3)C16−O15	BD*(2)C2−C3	0.25
LP(2)O12	BD*(3)C16−O15	1.21	LP(3)O17	LP(2)N1	0.21
LP(3)O12	BD*(3)C16−O15	0.92	LP(3)O17	BD*(3)S4−C5	0.21
			BD*(3)C16−O15	BD*(2)C2−C3	3.93
From CO_2[a] to CO_2[b]			From CO_2[c] to CO_2[b]		
BD(3)C10−O11	BD*(3)C13−O14	0.25	LP(1)O17	BD*(2)C13−O14	0.29
			LP(2)O17	BD*(2)C13−O14	1.30
			LP(3)O17	BD*(2)C13−O14	0.25

[a]The carbon atom number 10 of CO_2. [b]The carbon atom number 13 of CO_2. [c]The carbon atom number16 of CO_2. [d]BD for 2−center bond, LP for 1−center valence lone pair the unstarred and starred labels corresponding to Lewis and non−Lewis NBOs, respectively. [e]RY* for 1−center Rydberg, and BD* for 2−center antibond, the unstarred and starred labels corresponding to Lewis and non−Lewis NBOs, respectively.

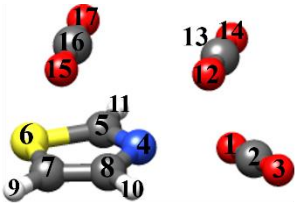

17
16
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Table S8. Experimental transition frequencies of the parent species of the thiazole-CO_2 complex.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$ (MHz)
4	0	4	3	3	0	3	2	5996.3870	−0.0027
4	0	4	4	3	0	3	3	5996.4686	0.0025
4	0	4	5	3	0	3	4	5996.5063	−0.0005
4	2	3	4	3	2	2	4	6024.8101	0.0011
4	2	3	5	3	2	2	2	6025.3666	−0.0008
4	2	3	3	3	2	2	3	6025.5088	−0.0001
4	2	2	4	3	2	1	3	6056.0019	0.0004
4	2	2	5	3	2	1	4	6056.5491	−0.0006
4	2	2	3	3	2	1	2	6056.6919	0.0006
4	1	3	3	3	1	2	3	6271.1175	0.0006
4	1	3	5	3	1	2	2	6271.2425	0.0021
4	1	3	5	3	1	2	4	6271.2793	0.0000
5	1	5	5	4	1	4	4	7208.8215	−0.0009
5	1	5	4	4	1	4	3	7208.8617	−0.0020
5	1	5	6	4	1	4	5	7208.9158	−0.0008
5	0	5	4	4	0	4	3	7472.4623	0.0022
5	0	5	5	4	0	4	4	7472.4934	−0.0017
5	0	5	6	4	0	4	5	7472.5278	−0.0009
5	2	4	5	4	2	3	4	7527.3569	0.0008
5	2	4	6	4	2	3	5	7527.6504	0.0014
5	2	4	4	4	2	3	3	7527.6774	−0.0012
5	3	3	5	4	3	2	4	7544.2975	−0.0004
5	3	3	6	4	3	2	5	7544.9227	−0.0014
5	3	3	4	4	3	2	3	7545.0804	0.0025
5	3	2	5	4	3	1	4	7545.3265	0.0003
5	3	2	6	4	3	1	5	7545.9516	−0.0004
5	3	2	4	4	3	1	3	7546.1074	0.0013
5	2	3	5	4	2	2	4	7589.3788	−0.0004
5	2	3	6	4	2	2	5	7589.6611	0.0011
5	2	3	4	4	2	2	3	7589.6871	−0.0012
5	1	4	5	4	1	3	4	7832.7101	−0.0013
5	1	4	4	4	1	3	3	7832.7659	0.0014
5	1	4	6	4	1	3	5	7832.7978	−0.0032
6	1	6	6	5	1	5	5	8642.6892	0.0025
6	1	6	5	5	1	5	4	8642.7085	0.0018
6	1	6	7	5	1	5	6	8642.7502	0.0033
6	0	6	5	5	0	5	4	8933.8802	−0.0009
6	0	6	6	5	0	5	5	8933.9003	0.0039

6	0	6	7	5	0	5	6	8933.9249	−0.0016
6	2	5	6	5	2	4	5	9027.1532	0.0021
6	2	5	5	5	2	4	4	9027.3276	0.0016
6	2	5	7	5	2	4	6	9027.3276	0.0015
6	3	4	6	5	3	3	5	9056.9356	−0.0040
6	3	4	7	5	3	3	6	9057.3073	0.0006
6	3	4	5	5	3	3	4	9057.3608	−0.0029
6	3	3	6	5	3	2	5	9059.6764	−0.0006
6	3	3	7	5	3	2	6	9060.0435	0.0001
6	3	3	5	5	3	2	5	9060.0977	−0.0026
6	2	4	6	5	2	3	5	9134.5868	0.0015
6	2	4	5	5	2	3	4	9134.7456	0.0011
6	2	4	7	5	2	3	6	9134.7456	−0.0002
6	1	5	6	5	1	4	5	9389.8264	0.0004
6	1	5	5	5	1	4	4	9389.8536	−0.0003
6	1	5	7	5	1	4	6	9389.8829	−0.0003
7	1	7	7	6	1	6	6	10072.6330	−0.0004
7	1	7	6	6	1	6	5	10072.6502	0.0055
7	1	7	8	6	1	6	7	10072.6732	−0.0023
7	0	7	7	6	0	6	6	10378.9527	−0.0001
7	0	7	6	6	0	6	5	10378.9527	0.0038
7	0	7	8	6	0	6	7	10378.9793	−0.0018
7	2	6	7	6	2	5	6	10523.7480	−0.0005
7	2	6	6	6	2	5	5	10523.8508	−0.0033
7	2	6	8	6	2	5	7	10523.8669	0.0040
7	3	5	7	6	3	4	6	10570.9685	−0.0006
7	3	5	8	6	3	4	7	10571.2049	0.0019
7	3	5	6	6	3	4	5	10571.2208	−0.0035
7	3	4	7	6	3	3	6	10577.1096	−0.0022
7	3	4	8	6	3	3	7	10577.3486	0.0040
7	3	4	6	6	3	3	5	10577.3636	−0.0021
7	2	5	7	6	2	4	6	10692.8578	−0.0043
7	2	5	6	6	2	4	5	10692.9436	−0.0067
7	2	5	8	6	2	4	7	10692.9660	0.0057
7	1	6	7	6	1	5	6	10941.3131	−0.0005
7	1	6	8	6	1	5	7	10941.3524	−0.0017
8	1	8	8	7	1	7	7	11498.3479	0.0000
8	1	8	7	7	1	7	6	11498.3579	0.0032
8	1	8	9	7	1	7	8	11498.3758	−0.0036
8	0	8	8	7	0	7	7	11807.0062	0.0043

8	0	8	7	7	0	7	6	11807.0062	0.0015
8	0	8	9	7	0	7	8	11807.0260	−0.0027
8	2	7	8	7	2	6	7	12016.6652	0.0012
8	2	7	7	7	2	6	6	12016.7307	−0.0022
8	2	7	9	7	2	6	8	12016.7486	0.0048
8	3	6	8	7	3	5	7	12086.3579	−0.0005
8	3	6	9	7	3	5	8	12086.5144	−0.0024
8	3	6	7	7	3	5	6	12086.5272	0.0039
8	3	5	8	7	3	4	7	12098.5943	0.0000
8	3	5	9	7	3	4	8	12098.7496	−0.0012
8	3	5	7	7	3	4	6	12098. 7496	−0.0074
8	2	6	8	7	2	5	7	12264.3396	0.0025
8	2	6	7	7	2	5	6	12264.3817	−0.0058
8	2	6	9	7	2	5	8	12264.4020	0.0025
8	1	7	8	7	1	6	7	12485.8632	−0.0019
8	1	7	9	7	1	6	8	12485.8935	−0.0028
9	0	9	9	8	0	8	8	13218.6570	0.0009
9	0	9	8	8	0	8	7	13218.6662	0.0031
9	0	9	10	8	0	8	9	13218.6786	−0.0032
9	2	8	9	8	2	7	8	13505.4145	0.0015
9	2	8	10	8	2	7	9	13505.4759	0.0041
9	3	7	9	8	3	6	8	13602.9205	0.0020
9	3	7	8	8	3	6	7	13603.0323	0.0016
9	3	7	10	8	3	6	9	13603.0323	0.0014
9	3	6	9	8	3	5	8	13625.2161	−0.0027
9	3	6	8	8	3	5	7	13625.3298	0.0015
9	3	6	10	8	3	5	9	13625.3298	0.0012
9	2	7	9	8	2	6	8	13847.8336	0.0067
9	2	7	8	8	2	6	7	13847.8530	−0.0029
9	2	7	10	8	2	6	9	13847.8718	0.0042
9	1	8	9	8	1	7	8	14021.9978	−0.0056
9	1	8	10	8	1	7	9	14022.0311	0.0019
10	1	10	10	9	1	9	9	14336.4464	−0.0029
10	1	10	9	9	1	9	8	14336.4464	−0.0073
10	1	10	11	9	1	9	10	14336.4731	0.0033
10	0	10	10	9	0	9	9	14615.7857	−0.0050
10	0	10	9	9	0	9	8	14615.7926	−0.0073
10	0	10	11	9	0	9	10	14615.8170	0.0018
10	2	9	10	9	2	8	9	14989.5321	0.0041
10	2	9	9	9	2	8	8	14989.5607	−0.0024

10	2	9	11	9	2	8	10	14989.5758	0.0027
10	3	8	10	9	3	7	9	15120.3201	0.0007
10	3	8	9	9	3	7	8	15120.3992	0.0002
10	3	8	11	9	3	7	10	15120.3992	−0.0028
10	3	7	10	9	3	6	9	15158.2347	0.0020
10	3	7	9	9	3	6	8	15158.3116	0.0031
10	3	7	11	9	3	6	10	15158.3116	−0.0002
10	2	8	10	9	2	7	9	15440.8481	−0.0026
10	2	8	9	9	2	7	8	15440.8660	−0.0014
10	2	8	11	9	2	7	10	15440.8838	0.0057
10	1	9	10	9	1	8	9	15548.0808	−0.0032
10	1	9	11	9	1	8	10	15548.1138	0.0071
11	1	11	11	10	1	10	10	15748.8331	−0.0002
11	1	11	10	10	1	10	9	15748.8331	−0.0043
11	1	11	12	10	1	10	11	15748.8530	0.0022
11	0	11	12	10	0	10	10	16001.2341	−0.0040
11	0	11	11	10	0	10	11	16001.2664	0.0055
11	2	10	11	10	2	9	10	16468.5724	0.0032
11	2	10	10	10	2	9	9	16468.5908	−0.0055
11	2	10	12	10	2	9	11	16468.6046	−0.0006
11	3	9	11	10	3	8	10	16638.1030	−0.0022
11	3	9	12	10	3	8	11	16638.1647	−0.0032
11	3	8	11	10	3	7	10	16699.0189	0.0004
11	3	8	12	10	3	7	11	16699.0764	−0.0001
11	2	9	11	10	2	8	10	17039.9204	−0.0054
11	2	9	12	10	2	8	11	17039.9497	0.0049
11	1	10	11	10	1	9	10	17062.3139	−0.0046
11	1	10	12	10	1	9	11	17062.3437	0.0043
4	1	4	3	3	0	3	2	9151.9499	0.0012
4	1	4	4	3	0	3	3	9152.1046	−0.0019
4	1	4	5	3	0	3	4	9152.0834	0.0010
6	1	6	6	5	0	5	5	11534.6532	−0.0013
6	1	6	5	5	0	5	4	11534.6698	0.0006
6	1	6	7	5	0	5	6	11534.7102	0.0000
7	1	7	7	6	0	6	6	12673.3907	−0.0009
7	1	7	6	6	0	6	5	12673.4346	0.0018
7	1	7	8	6	0	6	7	12673.4580	−0.0013
8	1	8	8	7	0	7	7	13792.7852	−0.0014
8	1	8	7	7	0	7	6	13792.8393	0.0002
8	1	8	9	7	0	7	8	13792.8550	−0.0026

2	2	0	1	1	1	1	1	14303.2937	−0.0007
2	2	0	3	1	1	1	2	14304.4961	0.0012
2	2	0	2	1	1	1	1	14305.3405	−0.0009
2	2	0	2	1	1	1	2	14305.8086	−0.0022
9	1	9	9	8	0	8	8	14905.4252	−0.0001
9	1	9	8	8	0	8	7	14905.4766	−0.0037
9	1	9	10	8	0	8	9	14905.4985	0.0041
3	2	2	4	2	1	1	3	15558.1067	−0.0030
3	2	2	3	2	1	1	2	15558.3901	0.0002
3	2	2	2	2	1	1	1	15558.8946	0.0013
3	2	1	2	2	1	2	1	15948.4784	−0.0013
3	2	1	4	2	1	2	3	15948.9354	0.0022
3	2	1	3	2	1	2	2	15949.7527	−0.0003
10	1	10	10	9	0	9	9	16023.2184	−0.0001
10	1	10	9	9	0	9	8	16023.2717	0.0006
10	1	10	11	9	0	9	10	16023.2876	0.0053
4	2	3	3	3	1	2	2	16877.2217	−0.0020
4	2	3	5	3	1	2	4	16877.3841	0.0013
4	2	3	4	3	1	2	3	16877.6880	−0.0008
4	2	2	3	3	1	3	2	17673.7431	0.0017
4	2	2	5	3	1	3	4	17674.0160	−0.0004
4	2	2	4	3	1	3	3	17674.6589	−0.0011
5	2	4	4	4	1	3	3	18133.6634	0.0013
5	2	4	6	4	1	3	5	18133.7511	−0.0013
5	2	4	5	4	1	3	4	18133.9301	0.0033
6	2	5	5	5	1	4	4	19328.2241	0.0005
6	2	5	7	5	1	4	6	19328.2788	0.0013
6	2	5	6	5	1	4	5	19328.3638	−0.0026
5	2	3	4	4	1	4	3	19491.8653	0.0026
5	2	3	6	4	1	4	5	19492.0417	−0.0011
5	2	3	5	4	1	4	4	19492.5752	0.0013

Table S9. Experimental transition frequencies of the ^{13}C2 isotopic species of the thiazole-CO_2 complex.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$ (MHz)
4	0	4	3	3	0	3	2	5927.0614	−0.0061
4	0	4	4	3	0	3	3	5927.1462	0.0020
4	0	4	5	3	0	3	4	5927.1885	0.0038
5	1	5	5	4	1	4	4	7128.1468	−0.0008
5	1	5	4	4	1	4	3	7128.1888	0.0000
5	1	5	6	4	1	4	5	7128.2427	0.0009
5	0	5	4	4	0	4	3	7386.8877	0.0004
5	0	5	5	4	0	4	4	7386.9249	0.0023
5	0	5	6	4	0	4	5	7386.9535	−0.0024
6	0	6	5	5	0	5	4	8832.7086	0.0016
6	0	6	6	5	0	5	5	8832.7206	−0.0019
6	0	6	7	5	0	5	6	8832.7525	0.0001

Table S10. Experimental transition frequencies of the ^{13}C5 isotopic species of the thiazole-CO_2 complex.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$ (MHz)
4	0	4	4	3	0	3	3	5989.6134	−0.0036
4	0	4	5	3	0	3	4	5989.6578	0.0000
5	1	5	4	4	1	4	4	7199.4427	0.0047
5	1	5	6	4	1	4	3	7199.4797	0.0004
5	1	5	4	4	1	4	5	7199.5347	0.0025
5	0	5	4	4	0	4	3	7463.5646	0.0019
5	0	5	5	4	0	4	4	7463.5998	0.0021
5	0	5	6	4	0	4	5	7463.6311	−0.0002
6	1	6	6	5	1	5	5	8631.3136	−0.0015
6	1	6	7	5	1	5	6	8631.3704	−0.0049
6	0	6	5	5	0	5	6	8922.7361	−0.0027
6	0	6	6	5	0	5	4	8922.7586	0.0046
6	0	6	7	5	0	5	5	8922.7817	−0.0025

Table S11. Experimental transition frequencies of the ^{34}S6 isotopic species of the thiazole-CO_2 complex.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$ (MHz)
5	1	5	5	4	1	4	4	7089.5335	−0.0056
5	1	5	4	4	1	4	3	7089.5899	0.0095
5	1	5	6	4	1	4	5	7089.6301	−0.0031
5	0	5	4	4	0	4	3	7347.1043	0.0010
5	0	5	5	4	0	4	4	7347.1398	0.0012
5	0	5	6	4	0	4	5	7347.1668	−0.0052
6	1	6	6	5	1	5	5	8499.9126	−0.0026
6	1	6	5	5	1	5	4	8499.9374	0.0022
6	1	6	7	5	1	5	6	8499.9711	−0.0042
6	0	6	5	5	0	5	4	8785.0049	−0.0014
6	0	6	6	5	0	5	5	8785.0282	0.0062
6	0	6	7	5	0	5	6	8785.0500	−0.0018
7	1	7	7	6	1	6	6	9906.5454	−0.0008
7	1	7	6	6	1	6	5	9906.5624	0.0049
7	1	7	8	6	1	6	7	9906.5913	0.0029
7	0	7	7	6	0	6	6	10207.2626	0.0021
7	0	7	6	6	0	6	5	10207.2626	0.0064
7	0	7	8	6	0	6	7	10207.2826	−0.0058
8	1	8	8	7	1	7	7	11309.1268	0.0027
8	1	8	7	7	1	7	6	11309.1335	0.0022
8	1	8	9	7	1	7	8	11309.1475	−0.0080
8	0	8	8	7	0	7	7	11613.1474	−0.0065
8	0	8	7	7	0	7	6	11613.1474	0.0039
8	0	8	9	7	0	7	8	11613.1655	−0.0021
9	0	9	10	8	0	8	9	13003.1642	−0.0019

Table S12. Experimental transition frequencies of the ^{13}C7 isotopic species of the thiazole-CO_2 complex.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$ (MHz)
5	1	5	5	4	1	4	4	7152.2206	−0.0011
5	1	5	4	4	1	4	3	7152.2614	−0.0016
5	1	5	6	4	1	4	5	7152.3152	−0.0007
5	0	5	4	4	0	4	3	7414.1613	0.0011
5	0	5	5	4	0	4	4	7414.1940	−0.0011
5	0	5	6	4	0	4	5	7414.2224	−0.0064
6	1	6	6	5	1	5	5	8574.7758	0.0012
6	1	6	5	5	1	5	4	8574.7982	0.0036
6	1	6	7	5	1	5	6	8574.8340	−0.0007
6	0	6	7	5	0	5	4	8863.9562	−0.0004
6	0	6	5	5	0	5	5	8863.9767	0.0048
6	0	6	6	5	0	5	6	8864.0007	−0.0013
6	1	5	6	5	1	4	5	9317.7367	−0.0009
6	1	5	5	5	1	4	4	9317.7683	0.0026
6	1	5	7	5	1	4	6	9317.7945	−0.0004

Table S13. Experimental transition frequencies of the ^{13}C8 isotopic species of the thiazole-CO_2 complex.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$ (MHz)
4	1	3	3	3	1	2	2	6260.6609	−0.0021
4	1	3	5	3	1	2	4	6260.7030	0.0010
5	1	5	5	4	1	4	4	7187.9424	−0.0006
5	1	5	4	4	1	4	3	7187.9814	−0.0030
5	1	5	6	4	1	4	5	7188.0360	−0.0013
5	1	4	4	4	1	3	3	7819.2617	0.0022
5	1	4	6	4	1	3	5	7819.2934	−0.0026
6	1	6	6	5	1	5	5	8617.3089	−0.0007
6	1	6	5	5	1	5	4	8617.3348	0.0050
6	1	6	7	5	1	5	6	8617.3701	0.0001
6	0	6	5	5	0	5	4	8909.3935	−0.0024
6	0	6	6	5	0	5	5	8909.4147	0.0038
6	0	6	7	5	0	5	6	8909.4394	−0.0019
6	1	5	6	5	1	4	5	9373.1854	0.0023
6	1	5	5	5	1	4	4	9373.2103	−0.0008
6	1	5	7	5	1	4	6	9373.2403	−0.0001