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Supplementary information for:

Unexpected discovery of estrone in the rotational spectrum of estradiol: A systematic investigation of a CP-FTMW spectrum

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Abstract

We report the reinvestigation of the high-resolution rotational spectrum of estradiol. After removing the known spectral lines corresponding to three conformers of estradiol identified in the gas phase before, a large number of spectral lines remained unassigned in the spectrum. The observation of remaining lines is a common feature in spectra obtained by broadband rotational spectroscopy. In our reinvestigation, the detection of certain patterns resulted in two new sets of experimental rotational constants. Here we describe a systematic analysis, which together with quantum-chemical computations culminated in the assignment of two estrone conformers, namely exhibiting the *trans*- and the *cis*-arrangement of the hydroxy group attached to the rigid steroid backbone. Estrone and estradiol only differ in two atomic mass units, and they show a dynamic interconversion equilibrium under certain conditions, which might also have been the case in our experiments due to the heating temperature of 195°C. The results illustrate the potential of high-resolution rotational spectroscopy to discern between structurally related molecules and to provide their gas-phase structures without information beforehand exploiting the benefit of having remaining unassigned rotational transitions in the spectrum.

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Figure S1. The 16 different diastereomers of estradiol. The corresponding enantiomer would have the opposite configuration for the five chiral centers and, thus, would have the same set of rotational constants. Estradiol-*17β* (RSSSS) and the diastereomer RSRSR are highlighted with dashed boxes.

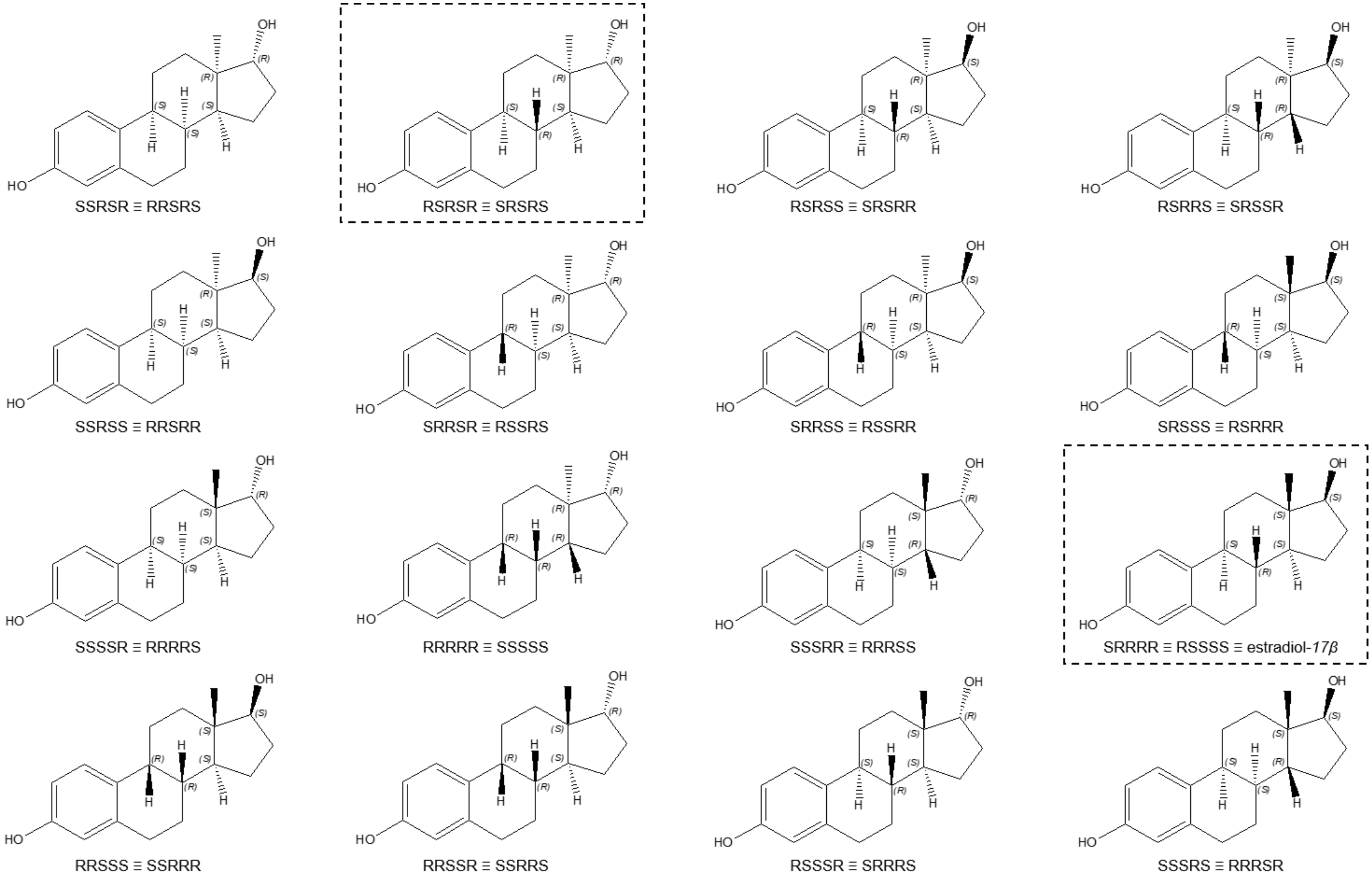

Figure S2. The two configurations of estrone, showing the *trans* and *cis* arrangements of their OH groups.

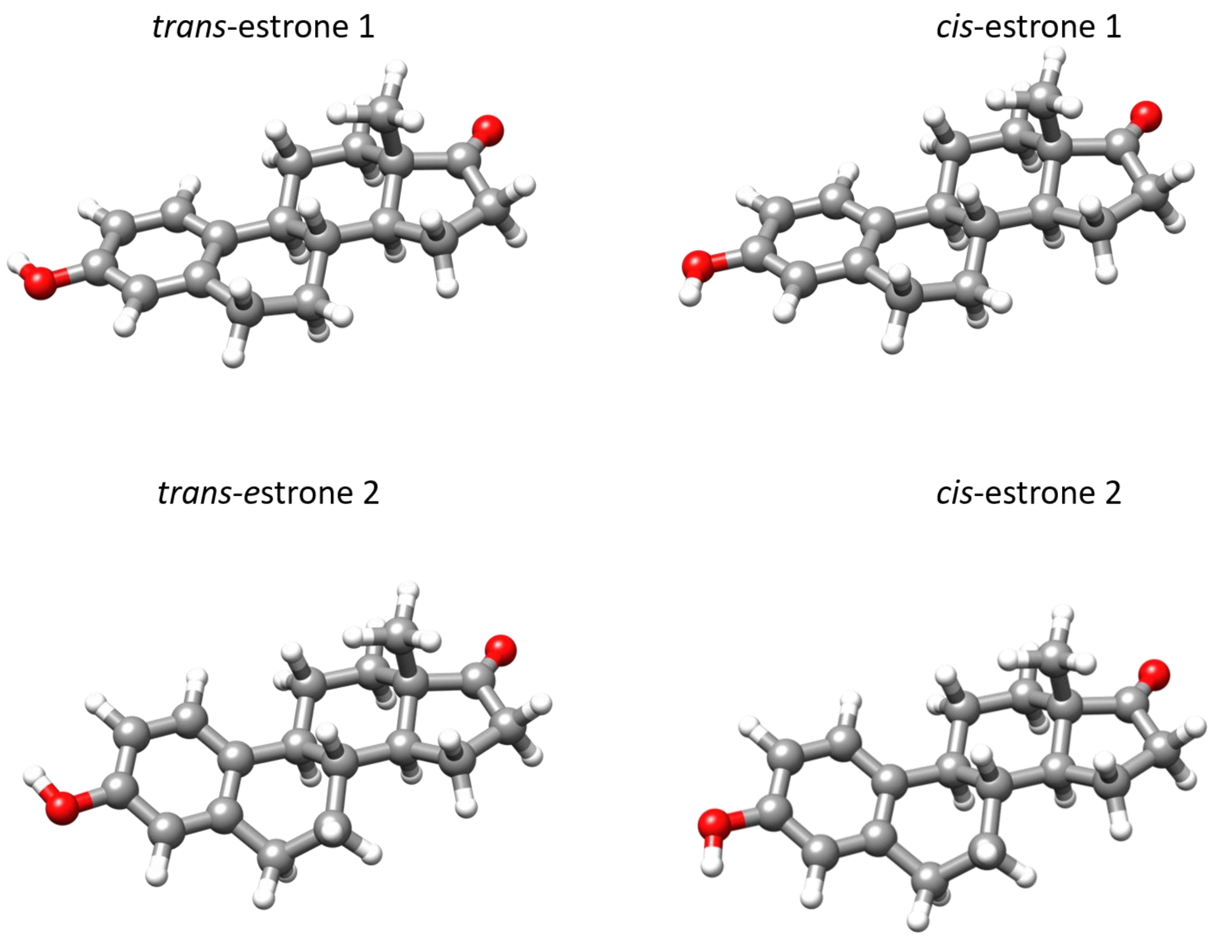

Figure S3. Overlay of the *trans* forms for estrone 1 (blue atoms) and estrone 2 (gold atoms) to illustrate the differences in their backbones.

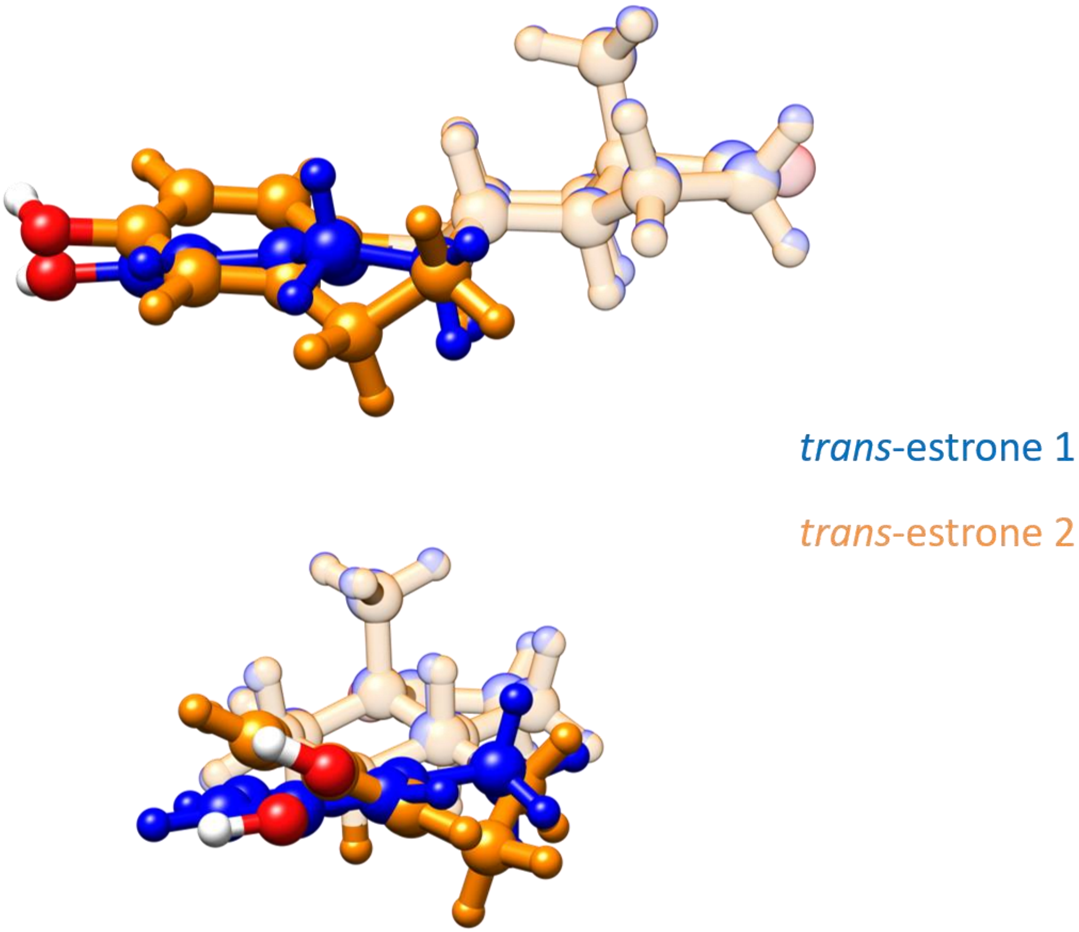

Table S1. Predicted rotational parameters for the 16 estradiol diastereomers at the B3LYP-D3(BJ)/def2-TZVP level of theory named by the configuration (R or S) of the five chiral centers (C8-C9-C13-C14-C17, Figure 1 for atom labelling). A conformational search was performed by CREST for each diastereomer, and only the lowest energy rotamer was optimized and shown in this table. The name of the rotamer is given according to the orientation of both -OH groups, t and c stands for *trans* and *cis* respectively, gp, gm and a stand for *gauche(+)*, *gauche(-)* and *anti*, respectively. The diastereomers highlighted in pale orange have been synthesized previously [Reference 26 in manuscript]. Rotational constants highlighted in pale green mean those are similar to the experimental rotational constants for new-a and new-b. Only two structures fulfill both criteria, RSSSS (estradiol-*17β*) and RSRSR.

Configuration	SRRSS	SRRSR	RRRSS	RRRSR	RSSSR estradiol-*17α*	RSSSS estradiol-*17β*	RSRSR	RSRSS
Rotamer	ca	tgp	ca	tgp	tgp	tgp	ca	ta
A /MHz[a]	903.5	938.3	926.3	968.9	906.4	943.7	945.3	886.0
B /MHz	177.1	176.0	175.4	175.0	179.5	175.0	177.7	180.0
C /MHz	163.2	164.0	167.6	167.3	161.6	155.4	159.4	160.6
B-C /MHz	13.9	12.0	7.8	7.7	17.9	19.6	18.2	19.4
P_a /uÅ^2	2695.5	2707.2	2675.5	2693.5	2694.4	2802.4	2739.9	2692.0
P_b /uÅ^2	401.2	374.4	339.8	327.3	434.9	449.4	430.6	454.8
P_c /uÅ^2	158.1	164.2	205.7	194.4	122.7	86.2	104.1	115.6
$\mu_a\|\mu_b\|\mu_c$ /D	-0.94|-1.79|-0.35	1.02|-0.43|-1.00	-0.85|-1.23|-0.71	1.03|1.20|-0.93	-0.56|0.17|-0.33	1.13|-2.41|-0.79	0.07|-0.35|0.21	0.88|-0.26|-0.26
R $\mu_a\|\mu_b\|$	0.53|1	1|0.42	0.69|1	0.86|1	1|0.30	0.47|1	0.21|1	1|0.30

Configuration	RRSRR	RRRRS	RRRRR	RRSSR	RRSSS	RRSRS	SRSSR	SRSSS
Rotamer	tgp	ta	tgp	ta	tgp	ta	tgp	ta
A /MHz	624.7 / 860.8[b]	943.7	994.8	605.2 / 919.0[b]	635.9 / 963.2[b]	888.3	889.3	957.2
B /MHz	243.2 / 196.1	179.2	173.1	236.6 / 179.6	220.3 / 174.6	185.1	184.1	177.1
C /MHz	219.1 / 181.2	164.6	159.7	230.9 / 163.6	209.9 / 155.8	170.9	168.1	162.5
B-C /MHz	24.1	14.6	13.5	5.8	10.4	14.2	15.9	14.6
P_a /uÅ^2	1788.7	2679.2	2789.0	1745.2	1953.5	2559.3	2592.4	2717.8
P_b /uÅ^2	518.9	393.0	377.5	444.4	454.2	397.9	414.0	392.2
P_c /uÅ^2	290.2	142.6	130.5	390.8	340.5	171.0	154.2	135.8
$\mu_a\|\mu_b\|\mu_c$ /D	1.69|1.92|0.59	-0.52|-0.26|-0.47	-0.43|0.35|-0.20	-0.10|0.69|-1.42	0.12|-0.37|1.53	0.39|0.74|-1.88	0.39|0.24|0.36	-0.35|-0.33|0.10
R $\mu_a\|\mu_b\|$	0.88|1	1|0.50	1|0.81	0.14|1	0.32|1	0.53|1	1|0.62	1|0.94

[a] *A*, *B* and *C* are the rotational constants. P_α (α = *a*, *b* or *c*) are the planar moments of inertia; $P_a = (I_b+I_c-I_a)/2$. μ_α (α = *a*, *b* or *c*) are the electric dipole moment components, 1 D = 3.33·10^{-30} C·m. R $\mu_a|\mu_b$ is the ratio of the dipole moment components estimated from quantum-chemical calculations. [b] For the RRSRR, RRSSR and RRSSS diastereomers the CREST search predicted two conformations for the backbone close in energy. The lowest in energy has a "non-planar" backbone, which explains the large difference in the rotation constants relative to the other diastereomers. The "planar" backbone structure was also considered, their rotational constants are shown in the table after the slash. The planar moments of inertia and the dipole moment components are given for the lowest energy structure, the "non-planar" one.

Table S2. Predicted rotational parameters for the six rotamers of estradiol RSRSR at the B3LYP-D3(BJ)/def2-TZVP level of theory. The rotamers are sorted by increasing energy, note that the order is different to the rotamers of estradiol-*17β*.

	Cis-anti (ca)	*Trans-anti* (ta)	*cis-gauche(-)* (cgm)	*trans-gauche(-)* (tgm)	*trans-gauche(+)* (tgp)	*cis-gauche(+)* (cgp)
A /MHz[a]	945.3	945.8	944.6	945.1	944.7	944.2
B /MHz	177.7	177.6	178.0	178.0	177.5	177.5
C /MHz	159.4	159.4	159.8	159.8	159.3	159.3
B-C /MHz	18.2	18.2	18.2	18.2	18.2	18.2
P_a /uÅ^2	2739.9	2740.9	2733.4	2733.5	2742.4	2742.2
P_b /uÅ^2	430.6	429.6	429.2	429.1	430.1	430.3
P_c /uÅ^2	104.1	104.7	105.8	105.7	104.8	105.0
μ_a|μ_b|μ_c /D	0.07|-0.35|0.21	0.29|-2.19|-0.10	-1.09|1.95|-1.31	0.87|-0.58|-1.22	0.90|-0.10|-0.05	0.68|2.44|-0.15
R μ_a|μ_b|	0.21|1	0.13|1	0.56|1	1|0.67	1|0.11	0.28|1
ΔE_{ZPE} /cm^{-1}	0.00	10.89	131.16	135.27	337.17	340.15
ΔE_{ZPE} /kJ·mol^{-1}	0.00	0.13	1.57	1.62	4.03	4.07

[a] see Table S1 for definitions.

Table S3. Predicted rotational parameters for the two estrone conformations at the B3LYP-D3(BJ)/def2-TZVP level of theory. Each of the conformations presents two forms, *trans* or *cis,* due to the arrangement of the OH group at C3.

	Trans-estrone 1	*Cis*-estrone 1	*Trans*-estrone 2	*Cis*-estrone 2
A /MHz[a]	943.4	943.0	918.8	918.5
B /MHz	179.7	179.6	183.1	183.1
C /MHz	159.2	159.2	163.6	163.6
B-C /MHz	20.5	20.5	19.5	19.5
P_a /uÅ^2	2725.6	2725.9	2649.0	2649.8
P_b /uÅ^2	448.7	448.8	439.5	439.8
P_c /uÅ^2	87.0	87.1	110.5	110.4
$\mu_a\|\mu_b\|\mu_c$ /D	1.91|-0.93|0.38	-1.72|3.46|0.74	-1.89|0.68|1.02	1.80|-3.21|0.65
R $\mu_a\|\mu_b\|$	1|0.49	0.50|1	1|0.36	0.56|1
ΔE_{ZPE} /cm^{-1}	0	21.93	580.94	631.81
ΔE_{ZPE} /kJ·mol^{-1}	0	0.26	6.95	7.56

[a] see Table S1 for definitions.

Table S4. Observed frequencies and residuals (MHz) for *trans*-estrone for $J'K'_{-1}K'_{+1} \leftarrow J''K''_{-1}K''_{+1}$ transitions.

$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.	$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.	$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.
8 0 8	7 0 7	2677.3885	-0.0030	16 1 15	15 1 14	5494.9073	0.0070	17 2 15	16 2 14	5911.2794	-0.0067
9 0 9	8 0 8	3003.0854	-0.0030	17 1 17	16 1 16	5528.3414	-0.0014	18 2 17	17 2 16	6036.4162	-0.0043
10 0 10	9 0 9	3326.4033	-0.0032	17 1 16	16 1 15	5823.7090	0.0013	18 2 16	17 2 15	6261.0725	-0.0092
11 0 11	10 0 10	3647.5846	-0.0017	18 1 18	17 1 17	5848.7707	0.0063	19 2 18	18 2 17	6364.7638	-0.0023
12 0 12	11 0 11	3966.9825	-0.0017	18 1 17	17 1 16	6149.7808	0.0075	19 2 17	18 2 16	6609.0333	-0.0062
13 0 13	12 0 12	4285.0058	-0.0142	19 1 19	18 1 18	6168.8275	-0.0023	20 2 18	19 2 17	6954.9545	0.0125
14 0 14	13 0 13	4602.1216	0.0029	19 1 18	18 1 17	6473.1823	0.0133	21 2 20	20 2 19	7018.6920	-0.0015
16 0 16	15 0 15	5234.9518	0.0025	20 1 20	19 1 19	6488.5785	-0.0090	6 3 3	5 3 2	2035.0617	0.0031
17 0 17	16 0 16	5551.2106	0.0032	20 1 19	19 1 18	6794.0922	0.0033	8 3 6	7 3 5	2714.4995	0.0033
18 0 18	17 0 17	5867.5798	0.0022	21 1 21	20 1 20	6808.0778	-0.0051	8 3 5	7 3 4	2715.7629	0.0002
20 0 20	19 0 19	6500.9328	0.0019	21 1 20	20 1 19	7112.8388	-0.0035	9 3 7	8 3 6	3054.6689	-0.0049
21 0 21	20 0 20	6817.9586	0.0048	6 2 5	5 2 4	2030.8500	-0.0034	9 3 6	8 3 5	3056.9824	-0.0049
6 1 5	5 1 4	2090.5234	0.0089	6 2 4	5 2 3	2044.8980	0.0030	10 3 8	9 3 7	3395.0346	0.0033
7 1 7	6 1 6	2294.9999	-0.0095	7 2 6	6 2 5	2368.3079	0.0043	10 3 7	9 3 6	3398.9760	-0.0009
7 1 6	6 1 5	2437.2364	-0.0005	7 2 5	6 2 4	2390.5323	-0.0035	11 3 9	10 3 8	3735.5191	-0.0061
8 1 8	7 1 7	2621.0944	-0.0047	8 2 7	7 2 6	2705.2846	0.0023	11 3 8	10 3 7	3741.8903	-0.0023
8 1 7	7 1 6	2783.1080	0.0042	8 2 6	7 2 5	2738.1174	0.0031	12 3 10	11 3 9	4076.1021	0.0028
9 1 9	8 1 8	2946.5734	-0.0012	9 2 8	8 2 7	3041.7217	-0.0028	12 3 9	11 3 8	4085.9100	-0.0027
9 1 8	8 1 7	3127.9425	0.0014	9 2 7	8 2 6	3087.6185	0.0031	13 3 11	12 3 10	4416.6832	-0.0003
10 1 10	9 1 9	3271.4119	-0.0011	10 2 9	9 2 8	3377.5707	0.0032	13 3 10	12 3 9	4431.2234	-0.0029
10 1 9	9 1 8	3471.5535	-0.0019	10 2 8	9 2 7	3438.8740	0.0024	14 3 12	13 3 11	4757.2001	0.0027
11 1 11	10 1 10	3595.6042	-0.0020	11 2 10	10 2 9	3712.7517	0.0016	14 3 11	13 3 10	4778.0272	0.0038
11 1 10	10 1 9	3813.7381	0.0036	11 2 9	10 2 8	3791.5633	-0.0017	15 3 13	14 3 12	5097.5456	-0.0063
12 1 12	11 1 11	3919.1579	-0.0023	12 2 11	11 2 10	4047.2184	0.0032	15 3 12	14 3 11	5126.4785	0.0001
12 1 11	11 1 10	4154.2460	-0.0021	12 2 10	11 2 9	4145.2568	0.0002	16 3 14	15 3 13	5437.6610	0.0084
13 1 13	12 1 12	4242.0922	-0.0018	13 2 12	12 2 11	4380.9052	-0.0045	16 3 13	15 3 12	5476.7267	-0.0019
13 1 12	12 1 11	4492.8526	-0.0026	13 2 11	12 2 10	4499.4381	0.0005	17 3 15	16 3 14	5777.3908	-0.0102
14 1 14	13 1 13	4564.4365	-0.0009	14 2 13	13 2 12	4713.7877	0.0012	17 3 14	16 3 13	5828.8347	-0.0121
14 1 13	13 1 12	4829.3093	-0.0034	14 2 12	13 2 11	4853.5847	-0.0013	18 3 15	17 3 14	6182.8163	0.0030
15 1 15	14 1 14	4886.2328	0.0034	15 2 13	14 2 12	5207.2154	0.0004	19 3 17	18 3 16	6455.4536	0.0025
15 1 14	14 1 13	5163.3951	0.0031	16 2 15	15 2 14	5376.9292	-0.0013	20 3 18	19 3 17	6793.5638	0.0000
16 1 16	15 1 15	5207.5082	-0.0065	16 2 14	15 2 13	5559.9059	0.0061	22 3 20	21 3 19	7467.5304	-0.0062

Table S4. Continued.

$J' K'_{-1} K'_{+1}$	$J'' K''_{-1} K''_{+1}$	Obs.	Res.
6 4 3	5 4 2	2034.0526	-0.0100
6 4 2	5 4 1	2034.0526	-0.0100
7 4 4	6 4 3	2373.4805	-0.0033
7 4 3	6 4 2	2373.4805	-0.0033
9 4 6	8 4 5	3052.9299	0.0061
9 4 5	8 4 4	3052.9299	0.0061
10 4 7	9 4 6	3392.9428	-0.0105
10 4 6	9 4 5	3393.0445	0.0019
12 4 9	11 4 8	4073.8347	0.0041
12 4 8	11 4 7	4074.1701	0.0068
13 4 10	12 4 9	4414.6889	0.0027
13 4 9	12 4 8	4415.2740	-0.0015
14 4 11	13 4 10	4755.8284	-0.0018
15 4 12	14 4 11	5097.2701	0.0074
15 4 11	14 4 10	5098.8831	-0.0031
16 4 13	15 4 12	5438.9828	0.0072
16 4 12	15 4 11	5441.5242	-0.0045
17 4 14	16 4 13	5780.9584	0.0066
17 4 13	16 4 12	5784.8469	-0.0002
18 4 15	17 4 14	6123.1589	-0.0054
18 4 14	17 4 13	6128.9546	0.0057
9 5 5	8 5 4	3051.6945	0.0072
9 5 4	8 5 3	3051.6945	0.0072
10 5 6	9 5 5	3391.3055	0.0057
10 5 5	9 5 4	3391.3055	0.0057
11 5 7	10 5 6	3731.0947	0.0127
11 5 6	10 5 5	3731.0947	0.0127
12 5 8	11 5 7	4071.0500	-0.0014
12 5 7	11 5 6	4071.0500	-0.0014
15 5 11	14 5 10	5092.2397	-0.0181
15 5 10	14 5 9	5092.2397	-0.0181
6 1 6	5 0 5	2595.5561	-0.0006

$J' K'_{-1} K'_{+1}$	$J'' K''_{-1} K''_{+1}$	Obs.	Res.
7 1 7	6 0 6	2871.9202	-0.0083
8 1 8	7 0 7	3143.8108	0.0054
9 1 9	8 0 8	3412.9820	-0.0064
10 1 10	9 0 9	3681.3189	0.0057
11 1 11	10 0 10	3950.5146	0.0017
12 1 12	11 0 11	4222.0886	0.0018
13 1 13	12 0 12	4497.1923	-0.0042
14 1 14	13 0 13	4776.6177	0.0037
10 0 10	9 1 9	2916.5052	-0.0013
12 0 12	11 1 11	3664.0623	0.0045
16 0 16	15 1 15	5092.8879	0.0030
17 0 17	16 1 16	5436.5654	-0.0120
19 0 19	18 1 18	6111.2019	0.0139
6 2 5	5 1 4	4186.1726	0.0051
10 2 9	9 1 8	5240.2440	-0.0047
4 3 1	3 2 2	5200.6832	0.0044
5 3 3	4 2 2	5535.0034	0.0026
5 3 2	4 2 3	5541.2238	-0.0011
6 3 4	5 2 3	5868.6891	-0.0134
6 3 3	5 2 4	5883.2913	0.0061
7 3 5	6 2 4	6198.3399	0.0065
7 3 4	6 2 5	6227.5957	0.0033
8 3 6	7 2 5	6522.3022	0.0084
9 3 6	8 2 7	6926.7660	0.0094
10 3 8	9 2 7	7146.2834	0.0141
11 3 8	10 2 9	7648.3298	-0.0044
4 4 1	3 3 0	6737.4358	-0.0102
4 4 0	3 3 1	6737.4358	-0.0102
5 4 2	4 3 1	7076.2999	0.0015
5 4 1	4 3 2	7076.3283	-0.0058
6 4 3	5 3 2	7415.0038	-0.0050
6 4 2	5 3 3	7415.1466	-0.0060

$J' K'_{-1} K'_{+1}$	$J'' K''_{-1} K''_{+1}$	Obs.	Res.
7 4 4	6 3 3	7753.4280	-0.0030
7 4 3	6 3 4	7753.8662	0.0024

Table S5. Observed frequencies and residuals (MHz) for *cis*-estrone for $J'K'_{-1}K'_{+1} \leftarrow J''K''_{-1}K''_{+1}$ transitions.

$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.	$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.	$J'K'_{-1}K'_{+1}$	$J''K''_{-1}K''_{+1}$	Obs.	Res.
10 0 10	9 0 9	3325.8938	-0.0071	17 3 15	16 3 14	5776.5313	-0.0106	6 2 5	5 1 4	4184.6514	-0.0018
11 0 11	10 0 10	3647.0249	-0.0064	13 4 10	12 4 9	4414.0257	-0.0066	7 2 6	6 1 5	4462.4144	0.0082
12 0 12	11 0 11	3966.3901	0.0095	13 4 9	12 4 8	4414.6241	0.0018	8 2 7	7 1 6	4730.4192	0.0016
13 0 13	12 0 12	4284.3531	-0.0156	15 4 12	14 4 11	5096.5120	0.0030	9 2 8	8 1 7	4989.0066	-0.0005
15 0 15	14 0 14	4917.9129	-0.0034	16 4 12	15 4 11	5440.7303	0.0036	10 2 9	9 1 8	5238.6116	0.0067
7 1 6	6 1 5	2436.8600	-0.0071	13 5 9	12 5 8	4410.5674	-0.0040	10 2 8	9 1 9	6342.6084	-0.0140
8 1 7	7 1 6	2782.6944	0.0134	13 5 8	12 5 7	4410.5674	-0.0040	11 2 10	10 1 9	5479.7704	-0.0032
9 1 9	8 1 8	2946.1411	-0.0006	4 1 4	3 0 3	2022.3624	0.0039	13 2 12	12 1 11	5939.8759	0.0023
9 1 8	8 1 7	3127.4689	0.0038	5 1 5	4 0 4	2312.4217	0.0161	14 2 13	13 1 12	6160.7896	0.0007
15 1 15	14 1 14	4885.5108	0.0007	7 1 7	6 0 6	2871.2106	-0.0165	15 2 14	14 1 13	6377.2661	-0.0024
15 1 14	14 1 13	5162.5961	0.0036	8 1 8	7 0 7	3143.0754	0.0019	17 2 16	16 1 15	6803.0413	0.0054
12 2 10	11 2 9	4144.6500	-0.0001	9 1 9	8 0 8	3412.2321	0.0032	18 2 17	17 1 16	7015.7459	-0.0036
13 2 11	12 2 10	4498.7774	-0.0004	10 1 10	9 0 9	3680.5295	0.0012	19 2 18	18 1 17	7230.7430	-0.0044
14 2 13	13 2 12	4713.0794	-0.0004	11 1 11	10 0 10	3949.7071	0.0023	20 2 19	19 1 18	7449.7875	0.0157
14 2 12	13 2 11	4852.8669	-0.0051	12 1 12	11 0 11	4221.2525	-0.0045	21 2 20	20 1 19	7674.3773	-0.0108
15 2 13	14 2 12	5206.4283	-0.0174	13 1 13	12 0 12	4496.3451	-0.0010	22 2 21	21 1 20	7905.8689	-0.0123
16 2 14	15 2 13	5559.0738	-0.0009	14 1 14	13 0 13	4775.7491	0.0062	4 3 2	3 2 1	5196.3279	-0.0054
17 2 16	16 2 15	5706.2845	0.0016	15 1 15	14 0 14	5059.8485	0.0163	5 3 3	4 2 2	5532.6730	0.0027
17 2 15	16 2 14	5910.3978	-0.0068	16 1 16	15 0 15	5348.6395	-0.0240	5 3 2	4 2 3	5538.8956	0.0006
19 2 17	18 2 16	6608.0504	0.0071	17 1 17	16 0 16	5642.0419	0.0087	6 3 4	5 2 3	5866.3206	-0.0006
20 2 18	19 2 17	6953.8922	0.0044	18 1 18	17 0 17	5939.5603	-0.0034	6 3 3	5 2 4	5880.9090	0.0038
12 3 10	11 3 9	4075.5020	0.0074	24 1 24	23 0 23	7785.6289	0.0078	7 3 5	6 2 4	6195.8993	-0.0017
12 3 9	11 3 8	4085.3247	0.0130	13 0 13	12 1 12	4029.4884	-0.0039	7 3 4	6 2 5	6225.1620	-0.0005
13 3 11	12 3 10	4416.0263	-0.0019	14 0 14	13 1 13	4389.4392	-0.0042	8 3 6	7 2 5	6519.8142	0.0042
13 3 10	12 3 9	4430.5771	0.0008	16 0 16	15 1 15	5092.2397	-0.0049	8 3 5	7 2 6	6572.5732	0.0010
14 3 12	13 3 11	4756.4948	0.0034	18 0 18	17 1 17	5775.0354	-0.0048	9 3 7	8 2 6	6836.3183	0.0003
14 3 11	13 3 10	4777.3168	-0.0078	19 0 19	18 1 18	6110.3618	0.0076	9 3 6	8 2 7	6924.2307	0.0023
15 3 13	14 3 12	5096.7868	-0.0082	24 0 24	23 1 23	7747.7278	-0.0016	10 3 8	9 2 7	7143.6806	-0.0014
16 3 14	15 3 13	5436.8386	-0.0060	23 0 23	22 1 22	7423.9890	0.0030	10 3 7	9 2 8	7281.4369	0.0043
16 3 13	15 3 12	5475.9384	0.0050	5 2 4	4 1 3	3896.9186	-0.0120	11 3 9	10 2 8	7440.2815	-0.0027

Table S5. Continued.

$J' K'_{-1} K'_{+1}$	$J'' K''_{-1} K''_{+1}$	Obs.	Res.
11 3 8	10 2 9	7645.7092	-0.0014
12 3 10	11 2 9	7724.7715	0.0033
4 4 0	3 3 1	6734.3313	-0.0036
4 4 1	3 3 0	6734.3313	-0.0036
5 4 1	4 3 2	7073.1365	-0.0183
5 4 2	4 3 1	7073.1365	-0.0183
6 4 3	5 3 2	7411.7984	0.0013
6 4 2	5 3 3	7411.9344	-0.0064
7 4 3	6 3 4	7750.6125	0.0109
7 4 4	6 3 3	7750.1623	-0.0065
7 3 5	7 2 6	3856.1601	0.0072
8 3 6	8 2 7	3865.3817	0.0143
9 3 7	9 2 8	3878.3090	-0.0083
10 1 9	9 0 9	4794.1841	0.0132
14 1 13	13 0 13	6857.9917	0.0071
7 2 5	6 1 5	4512.8496	0.0074
9 2 7	8 1 7	5118.1866	0.0166
10 2 8	9 1 8	5429.0690	-0.0047