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re
28
re
28
re
29
ns
36

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Fig S2: The eight structures of AMPA optimized at the B3LYP-D3(BJ)/def2-TZVP level of theory along with their relative energies with and without zero-point energy (ZPE) correction in kJ/mol. The single-point energies obtained at DLPNO-CCSD/aug-cc-pVTZ level of theory along with single-point energies corrected with the zero-point energy term from the frequency calculations at the B3LYP-D3(BJ)/def2-TZVP level of theory are shown in red in the figure.



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Fig S8: Scan of the potential energy curve for the dihedral angles $\theta(O_{10}-C_8-C_7-O_{12})$ and $\varphi(H_{11}-O_{10}-C_8-C_7)$ at the B3LYP-D3(BJ)/def2-TZVP level of theory using ORCA for *cis-trans*, in-out motions of *trans*-out-perp. The position of the observed conformations is indicated in the plot and illustrated with the corresponding structure. See Figure S1 for atom labelling.



Fig S9: Scan of the potential energy curve for the dihedral angle $\tau(C_{13}-O_{12}-C_7-C_8)$ at the B3LYP-D3(BJ)/def2-TZVP level of theory using ORCA for par-perp motion of *trans*-in-par. The position of the observed conformations is indicated in the plot and illustrated with the corresponding structure. See Figure S1 for atom labelling.



Fig S10: The orange, black, and maroon traces show portions of rotational spectra obtained with He, Ne, and Ar carrier gases. The lower traces (in color) represent simulations employing the fitted rotational parameters of different conformers of AMPA as given in Table 2 of the manuscript.



Fig S11: Relaxed potential energy scans B3LYP-D3(BJ)/def2-TZVP for the internal rotation of the OCH₃ rotor for the conformers *cis*-out-par, *trans*-out-perp, and *cis*-out-perp. The experimental barrier for those three conformers could not be fitted.



Parameters	<i>cis</i> -in-perp	trans-out-par	<i>cis</i> -in-par	<i>cis</i> -out-par	trans-out-perp	cis-out-perp	<i>trans</i> -in-par	trans-in-perp
θ(O ₁₀ -C ₈ -C ₇ -O ₁₂)	5.9	-158.6	25.5	34.4	-153.9	37.9	172.0	164.9
φ(H ₁₁ -O ₁₀ -C ₈ -C ₇)	-3.1	-175.7	-3.3	176.5	-175.3	177.4	12.2	-11.1
$\tau(C_{13}-O_{12}-C_7-C_8)$	166.2	68.0	81.5	66.9	171.9	168.1	75.8	164.8

Table S1: Dihedral angles for three motions of eight conformers of AMPA calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory.

Table S2: Experimental rotational parameters obtained for the ¹³C isotopologues of the lowest energy conformer *cis*-in-perp obtained using SPFIT.

Parameters	Parent	¹³ C ₁	¹³ C ₂	¹³ C ₃	¹³ C ₄
A /MHz ^a	1436.68000(29)	1430.33229(39)	1432.23130(88)	1435.92383(68)	1429.22667(32)
<i>B</i> /MHz	692.06967(12)	689.06106(13)	684.44326(21)	682.27648(26)	685.34323(22)
C/MHz	583.21822(12)	581.79936(23)	577.99070(54)	576.32712(24)	579.44712(22)
⊿ı /kHz	0.07892(78)	[0.07892]	[0.07892]	[0.07892]	[0.07892]
$\varDelta_{ m JK}$ /kHz	0.3036(19)	0.3036(19)	0.425(40)	0.3036(19)	[0.3036]
$\Delta_{\rm K}$ /kHz	-0.0684(64)	[-0.0684]	[-0.0684]	[-0.0684]	[-0.0684]
$\delta_{ m J}$ /kHz	0.00462(13)	[0.00462]	[0.00462]	[0.00462]	[-0.00462]
δ_{κ} /kHz	-0.4362(24)	-0.426(34)	-0.74(11)	[-0.4362]	[-0.4362]
N ^b	248	27	23	21	25
σ /kHz	7.9	4.8	4.5	8.0	5.5

Parameters	¹³ C ₅	¹³ C ₆	¹³ C ₇	¹³ C ₈	¹³ C ₁₃
A /MHz	1431.48506(85)	1436.52869(48)	1435.42559(73)	1432.41928(61)	1409.04381(73)
<i>B</i> /MHz	690.21700(38)	691.78772(22)	690.92780(20)	689.25653(41)	690.30708(37)
C/MHz	582.39519(34)	583.09397(34)	582.60399(18)	580.53179(32)	577.99761(29)
⊿ı /kHz	[0.07892]	[0.07892]	[0.07892]	[0.07892]	[0.07892]
⊿ _{JK} /kHz	[0.3036]	[0.3036]	0.344(11)	[0.3036]	[0.3036]
⊿ _K /kHz	[-0.0684]	[-0.0684]	[-0.0684]	[-0.0684]	[-0.0684]
$\delta_{ m J}$ /kHz	[-0.00462]	[-0.00462]	[-0.00462]	[-0.00462]	[-0.00462]
$\delta_{ m K}$ /kHz	[-0.4362]	-0.461(32)	[-0.4362]	[-0.4362]	[-0.4362]
N	20	32	34	23	20
$\sigma/{ m kHz}$	7.9	7.2	6.1	7.9	9.8

[a] A, B, and C are the rotational constants. Δ_J , Δ_{JK} , Δ_K , δ_J and δ_K are the quartic centrifugal distortion constants. [b] N is the number of fitted transitions. σ is the root-mean-square deviation of the fit.

Parameters	<i>cis</i> -in-perp	trans-out-par
A /MHz ^a	1436.67998(15)	1619.14523(24)
<i>B</i> /MHz	692.06955(10)	635.06309(16)
C/MHz	583.21803(10)	570.21862(16)
⊿ _J /kHz	0.0782(60)	0.0731(1)
⊿ _{JK} /kHz	0.3081(11)	0.1412(23)
⊿ _K /kHz	-0.0797(44)	
$\delta_{ m j}$ /kHz	0.004664(92)	0.0046(12)
$\delta_{\rm K}$ /kHz	-0.4435(20)	0.8733(64)
a /b /c ^b	Y/Y/Y	N/Y/Y
V ₃ /kJmol ⁻¹	8.263(9)	7.552(2)
Nc	500	332
σ /kHz	7.7	8.5

Table S3: Experimental rotational parameters obtained using XIAM for the conformers *cis*-in-perp and *trans*-out-par.

[a] A, B, and C are the rotational constants. Δ_{J} , Δ_{JK} , Δ_{K} , δ_{J} and δ_{K} are the quartic centrifugal distortion constants. [b] Y and N indicates whether a, b or c type of rotational transitions were observed or not. [c] N is the number of fitted transitions. σ is the root-mean-square deviation of the fit.

Bond distance	r _o (Å)	r _s (Å)	r _e (Å)				
r(C2-C1)	1.399(62)	1.4037(14)	1.39				
r(C3-C2)	1.395(11)	1.4062(46)	1.39				
r(C4-C3)	1.3899(79)	1.3883(46)	1.39				
r(C5-C4)	1.3955(79)	1.4026(17)	1.39				
r(C6-C1)	1.398(15)	1.3470(45)	1.39				
r(C5-C6)	1.413(17)	1.4711(52)	1.39				
r(C7-C6)	1.467(14)	1.4542(38)	1.51				
r(C8-C7)	1.528(12)	1.495(15)	1.54				
r(O9-C8)	1.202(19)	-	1.20				
r(O10-C8)	1.367(14)	-	1.34				
r(012-C7)	1.435(12)	-	1.42				
r(C13-O12)	1.4255(89)		1.42				

Table S4: Experimentally determined bond distances, bond angles, and dihedral angles of conformer *cis*-in-perp using effectivestructure, r_0 , and substitution structure, r_s , method in comparison with the equilibrium, r_e , values obtained from quantum-
chemical calculations at the B3LYP-D3(BJ)/def2-TZVP level of theory.

Pond angles	r (°)	r (°)	r (°)
Bonu angles	I ₀ ()	I _s ()	r _e ()
$\Theta(C_3-C_2-C_1)$	120.31 (55)	119.94(17)	120.1
Θ(C ₄ -C ₃ -C ₂)	119.48(31)	119.42(10)	119.8
Θ(C ₅ -C ₄ -C ₃)	120.42(51)	120.76(18)	120.1
$\Theta(C_6-C_1-C_2)$	121.97(79)	122.49(23)	120.3
Θ(C ₇ -C ₆ -C ₁)	121.39(12)	123.29(47)	120.3
Θ(C ₈ -C ₇ -C ₆)	111.28(78)	112.42(88)	110.7
Θ(C ₄ -C ₅ -C ₆)	120.81(70)	119.18(20)	120.2
$\Theta(C_5-C_6-C_1)$	118.01(85)	117.97(25)	119.5
Θ(C ₅ -C ₆ -C ₇)	120.58(11)	118.70(43)	120.2
Θ(C ₆ -C ₇ -O ₁₂)	113.06(79)		113.1
Θ(C ₇ -O ₁₂ -C ₁₃)	114.09(51)		114.1
Θ(C ₇ -C ₈ -O ₁₀)	115.12(10)		115.1
Θ(C ₇ -C ₈ -O ₉)	122.06(83)		122.1
Θ(C ₈ -C ₇ -O ₁₂)	107.43(60)		107.6
Θ(O ₉ -C ₈ -O ₁₀)	122.82(12)		122.8

Dihedral angles	r _o (°)	r _s (°)	r _e (°)
Φ(C ₁ -C ₂ -C ₃ -C ₄)	-0.16(11)	-0.70(77)	-0.2
Φ(C ₁ -C ₆ -C ₇ -C ₈)	-94.86(12)	-100.64(66)	-95.1
$\Phi(C_2-C_3-C_4-C_5)$	-0.18(10)	-0.28(81)	-0.2
$\Phi(C_3-C_4-C_5-C_6)$	0.41(11)	-1.71(56)	0.4
$\Phi(C_4-C_5-C_6-C_7)$	-178.72(83)	-177.34(76)	-178.7
$\Phi(C_5-C_6-C_1-C_2)$	-0.07(14)	-5.94(33)	-0.1
$\Phi(C_6-C_1-C_2-C_3)$	0.29(12)	4.03(52)	0.3
$\Phi(C_5-C_6-C_7-C_8)$	83.54(11)	81.59(11)	83.3
Φ(C ₅ -C ₆ -C ₇ -O ₁₂)	-37.47(13)		-37.4

Φ(C ₆ -C ₇ -O ₁₂ -C ₁₃)	-71.35(96)	-71.4
Φ(C ₆ -C ₇ -C ₈ -O ₁₀)	-118.84(10)	-118.8
Φ(C ₆ -C ₇ -C ₈ -O ₉)	61.27(12)	61.3

							D:// /h /h /h
J	K′a	K′c	J″	K″a	K″c	Obs./MHz	Diff./MHz
1	1	1	0	0	0	2019.8957	-0.0009
6	2	4	6	1	5	2022.5574	0.0009
4	2	2	4	1	3	2035.1089	0.0002
Λ	1	4	2	2	1	2078 2844	-0.0024
2	2	1	2	1	2	2070.2044	0.0024
5	2	1	3	1	2	2132.5369	0.0043
7	2	5	7	1	6	2162.6566	0.0010
5	2	4	4	3	1	2316.2274	-0.0025
6	1	5	6	0	6	2401.2643	-0.0009
8	2	6	8	1	7	2426 0314	0.0019
2	1	2	1	1	1	2441 7165	0.0025
2	1	2	1	1	1	2441.7103	-0.0023
2	0	2	1	0	1	2539.4933	0.0038
2	1	1	1	1	0	2659.4259	0.0008
3	2	2	3	1	3	2730.2669	0.0021
9	2	7	9	1	8	2822.6073	0.0004
5	1	5	4	2	2	20/3 0003	-0.0061
4	2	2	-	4	2	2050 5125	0.0001
4	2	3	4	T	4	2959.5135	-0.0006
7	1	6	7	0	7	3015.2416	-0.0032
10	3	7	10	2	8	3018.0417	-0.0056
9	3	6	9	2	7	3061.8296	0.0104
8	4	5	7	5	2	3130 0999	-0.0037
2	-	2	, 2	1	2	2125 4220	0.0037
5	0	3	2	1	2	3135.4230	-0.0018
8	4	4	7	5	3	3148.1828	0.0081
2	1	2	1	0	1	3186.3268	-0.0012
8	3	5	8	2	6	3196.9323	-0.0018
4	1	3	3	2	2	3216 5496	-0.0014
	2	4	5	1	-	2249 6727	0.0010
10	2	4	10	2	10	3248.0737	-0.0010
12	3	9	12	2	10	3316.2248	0.0085
10	2	8	10	1	9	3349.6321	0.0065
7	3	4	7	2	5	3384.3888	0.0012
6	2	5	5	3	2	3496.1689	-0.0041
2	1	1	1	0	1	3512 8864	-0.0008
7	2	1	6	4	2	2556 5810	0.0000
/	3	4	0	4	5	3550.5810	0.0166
6	3	3	6	2	4	3581.9832	0.0001
6	2	5	6	1	6	3596.6371	0.0003
6	1	6	5	2	3	3652.8250	-0.0075
3	1	3	2	1	2	3655 9648	-0.0016
8	1	7	8	0	8	3691 5783	-0.0002
-	2	,	5	2	2	2752 2022	0.0002
5	3	2	5	2	3	3753.2932	-0.0031
3	0	3	2	0	2	3782.2679	0.0047
3	2	2	2	2	1	3825.8417	-0.0061
3	2	1	2	2	0	3869.4402	0.0004
4	3	1	4	2	2	3876 3620	0.0018
2	2	0	2	2	1	2047 8270	0.0196
2	3	2	2	2	1	3947.8279	0.0130
3	1	2	2	1	1	3981.8129	-0.0022
11	2	9	11	1	10	3987.9264	-0.0095
14	4	10	14	3	11	3996.7294	-0.0002
7	2	6	7	1	7	4000.1542	-0.0004
3	З	1	3	2	2	4001 7632	-0.0110
10	4	11	15	2	12	4006 6081	0.0010
15	4	11	15	3	12	4006.6981	0.0049
4	3	2	4	2	3	4030.6035	0.0001
4	3	1	4	2	3	4035.5515	0.0083
5	3	3	5	2	4	4086.4105	-0.0025
5	3	2	5	2	4	4105.9442	0.0018
13	4	<u> </u>	13	3	10	1119 2966	0.0072
13	4	5	13	2	2010	4119.2900	0.0072
6	2	4	5	3	3	4170.1252	0.0034
6	3	4	6	2	5	4179.0181	-0.0031
7	1	7	6	2	4	4187.5877	-0.0065
3	1	3	2	0	2	4302.8006	-0.0043
7	з	5	7	2	6	4317 3961	0.0029
12	4	0	12	2	0	4227 6902	0.0011
12	4	0	12	5	9	4337.0032	0.0011
Э	1	ð	9	U	Э	4390.2484	-0.0043
9	4	6	8	5	3	4445.8197	-0.0040
8	2	7	8	1	8	4453.8230	-0.0002
4	0	4	3	1	3	4476.0424	-0.0023
8	3	6	8	2	7	4508 7517	0.0014
7	2	с С	E S	2	2	4605 7620	-0.0027
/	2	о —	0	3	3	4005.7030	-0.0027
11	4	/	11	3	8	4606.6703	0.0036
8	3	6	7	4	3	4693.9085	0.0017
12	2	10	12	1	11	4704.4351	0.0030
5	1	4	4	2	3	4716.3585	0.0018
9	3	7	9	2	8	4757,9047	0.0005
1	1	Л	2	1	2	1863 2261	-0.0013
4	1	4	3	2	- -	4003.2201	-0.0013
10	4	6	10	3	/	48/9.825/	-0.0029

Table S5: Line list for the fit obtained using the SPFIT program for *cis*-in-perp conformer, measured rotational transitions are shown as Obs. and the residuals are shown as Diff.

2	2	1	1	1	0	4893.2482	-0.0010
9	2	8	9	1	9	4950.5300	-0.0032
3	1	2	2	0	2	4955.2039	-0.0090
8	3	5	7	4	4	4989.2646	-0.0003
2	2	0	1	1	1	5013.1965	0.0103
10	3	8	10	2	9	5066.8451	0.0056
4	2	3	3	2	2	5092,4746	-0.0020
10	1	9	10	0	10	5101 6937	0.0005
4	3	2	3	a a	1	5121 3132	0.0073
1	3	1	3	3	0	5125 5311	-0.00/7
4	2	2	3	2	1	5196 9813	-0.0047
4	1	2	2	1	2	5190.9813	-0.0020
4	1	3	5	2	2	5254.4005	-0.0010
0	4	4	°	3	2	5303.8702	0.0050
4	Ţ	4	3	0	3	5383.7664	-0.0026
	4	3	/	3	4	5429.8799	0.0059
11	3	9	11	2	10	5434.5/13	0.0004
10	2	9	10	1	10	5482.2591	-0.0041
6	4	2	6	3	3	5506.8924	0.0018
5	4	1	5	3	2	5549.2693	0.0144
7	4	4	7	3	5	5562.4151	0.0064
6	4	3	6	3	4	5562.5949	0.0004
5	4	2	5	3	3	5568.4415	-0.0050
4	4	0	4	3	1	5570.1620	0.0012
4	4	1	4	3	2	5575.0611	-0.0018
8	4	5	8	3	6	5575.1953	0.0087
8	4	4	8	3	6	5593.1513	0.0121
9	4	6	9	3	7	5610.0911	-0.0021
8	2	7	7	3	4	5615 0282	-0.0024
10	4	7	10	3	8	5677 2291	0.0024
7	2	5	6	3	1	5734 7742	0.0013
10	4	7	0	5	4	5765 2021	0.0025
10	4	,	11	2	4	5705.3521	0.0185
11	4	0	11	3	9	5780.4978	0.0024
11	1	10	11	0	11	5/92.19/4	0.0054
5	0	5	4	1	4	5795.4563	0.0021
12	3	10	12	2	11	5857.3255	0.0109
10	4	6	9	5	5	5869.8355	0.0136
9	3	7	8	4	4	5944.4489	-0.0090
11	2	10	11	1	11	6040.9650	-0.0078
3	2	2	2	1	1	6059.6670	-0.0049
5	1	5	4	1	4	6062.6110	-0.0015
3	2	1	2	1	1	6114.3419	-0.0058
14	5	9	14	4	10	6158.2334	0.0009
13	4	10	13	3	11	6163.6748	-0.0040
5	0	5	4	0	4	6182.6342	-0.0027
14	2	12	14	1	13	6221.4289	0.0034
6	1	5	5	2	4	6233.9612	-0.0171
13	3	11	13	2	12	6328.9923	0.0010
5	2	4	4	2	3	6351.7760	0.0030
3	2	2	2	1	2	6386.2347	0.0034
5	4	2	4	4	1	6400 9596	-0.0066
5	4	1	4	4	0	6401 2665	0.0002
5	2	2	4	2	2	6407 5867	0.0002
5	2	2	4	2	1	6422 1644	-0.0079
2	2	1	4 2	1	2	6440 0065	-0.0075
5	1	5	2	0	2	6440.3003	-0.0005
12	-	5	4	0	4	6449.7942	-0.0009
13	5	8	13	4	9	6456.0543	-0.0206
12	1	11	12	0	12	6463.0911	0.0150
4	1	3	3	0	3	6467.3634	0.0059
9	2	8	8	3	5	6490.4228	0.0038
9	3	6	8	4	5	6498.6875	0.0049
5	2	3	4	2	2	6545.2421	0.0060
5	1	4	4	1	3	6592.2835	0.0011
12	2	11	12	1	12	6619.3518	-0.0084
12	5	7	12	4	8	6692.3485	0.0097
14	3	12	14	2	13	6841.9987	-0.0024
11	5	6	11	4	7	6864.7828	0.0005
10	5	5	10	4	6	6982.7622	-0.0192
12	5	8	12	4	9	7052.2776	0.0018
9	5	4	9	4	5	7059.8701	-0.0162
11	5	7	11	4	8	7060.7625	0 0014
13	5	9	13	۵	10	7063 7302	0.0014
10	5	6	10	4	7	7080 2649	0.0014
6	0	6	10	1	5	7081 3854	-0.0120
11	1	0	10	с Г	5	7001.3034	-0.0024
11 7	4	õ	10	5 1	2	7006 7090	-0.0287
/	T	0	b	2	4	7096.7089	-0.008/
9	5	5	9	4	6	/103.6/51	-0.0070
14	5	10	14	4	11	/105.1948	0.0018

8	5	3	8	4	4	7108.7229	-0.0046
13	1	12	13	0	13	7116.2136	0.0059
8	5	4	8	4	5	7126.1615	-0.0095
7	5	2	7	4	3	7138.9927	0.0030
7	5	3	7	4	4	7144.9624	0.0070
10	3	8	9	4	5	7148.0324	0.0004
6	5	1	6	4	2	7157.3615	0.0215
6	5	2	6	4	3	7158.9927	-0.0048
5	5	0	5	4	1	7168.1100	-0.0059
5	5	1	5	4	2	/168.4451	-0.0068
4	2	3	3	1	2	/1/0.331/	-0.0017
15	5	11	15	4	12	/186.892/	0.0013
10	2	9	9	3	6	7200.5676	-0.0053
13	2	12	13	1	13	7211.3235	-0.01/1
°	2	6	,	3	4	7210.1222	0.0015
0 11	1	0	5 10		5	7254.1003	0.0069
11	4	2	2	1	2	7237.3482	-0.0104
4	2	2	5	1	5	7329.5141	-0.0024
8	2	6	7	3	5	7354 7456	0.0048
6	1	6	5	0	5	7521 3157	0.0001
6	2	5	5	2	4	7602 1189	0.0042
6	5	2	5	5	1	7679 4205	0.0033
6	5	1	5	5	0	7679 4205	-0 0149
6	4	3	5	4	2	7688.8975	0.0258
6	4	2	5	4	1	7690.2119	0.0006
6	3	4	5	3	3	7694.7486	0.0250
11	2	10	10	3	7	7724.0501	-0.0016
6	3	3	5	3	2	7732.5715	-0.0040
7	1	6	6	2	5	7751.1386	0.0016
14	1	13	14	0	14	7755.7596	0.0264
14	2	13	14	1	14	7812.2060	-0.0069
3	3	1	2	2	0	7816.5341	-0.0042
3	3	0	2	2	0	7817.2559	0.0078
4	2	3	3	1	3	7822.7485	0.0070
3	3	0	2	2	1	7828.3411	0.0092
6	1	5	5	1	4	7869.3891	-0.0055
6	2	4	5	2	3	7903.8830	-0.0057
4	2	2	3	1	3	7981.9213	-0.0032
6	3	3	5	4	2	2183.6638	0.0053
2	2	0	2	1	1	2244.9148	0.0069
5	2	3	4	3	2	2673.8168	0.0011
11	3	8	11	2	9	3095.9666	-0.0113
7	3	5	6	4	2	3416.2827	0.0145
13	3	10	13	2	11	3689.1646	-0.0037
10	5	6	9	6	3	4122.2482	-0.0058
10	5	5	9	6	4	4127.4985	-0.0057
14	3	11	14	2	12	4212.0998	0.0074
/	3	5	/	2	5	3245.7720	0.0031
0 6	2	0	0 6	2	4	2507.0018	0.0017
4	2	4	0	2	4	3324.3303	-0.0033
2	2	2	4	2	2	4002 5027	-0.0001
5	3	3	5	2	5	4002.3037	-0.0197
6	2	4	6	1	6	4251 0537	-0.0025
11	4	8	11	3	8	4397 0539	-0.0026
7	3	4	7	2	6	4456 0175	0.0056
8	1	8	7	2	5	4545.5989	0.0040
5	1	4	4	2	2	4557.1749	0.0012
8	3	6	7	4	4	4699.9884	-0.0024
11	1	11	10	2	8	4701.1428	0.0166
5	0	5	4	1	3	4711.8573	-0.0085
9	1	9	8	2	6	4736.8302	0.0103
7	1	7	6	2	5	4842.0117	-0.0019
3	0	3	2	1	1	2808.8588	-0.0067
4	1	3	3	2	1	3161.8723	-0.0029
6	1	6	5	2	4	4005.4751	-0.0036
15	3	12	15	2	13	4865.8176	0.0066
4	0	4	3	0	3	4996.5749	-0.0115
9	4	6	9	3	6	5073.8270	0.0058
12	6	7	11	7	4	5110.7185	-0.0083
12	6	6	11	7	5	5112.1809	-0.0034
9	4	5	9	3	6	5119.3669	-0.0134
8	4	5	8	3	5	5285.9113	-0.0012
9	3	6	9	2	8	5294.1543	-0.0219
16	3	13	16	2	14	5615.8259	-0.0158
8	1	8	7	2	6	5617.2179	-0.0014

7	2	5	6	3	3	5677.3940	0.0041
6	1	5	5	2	3	5881.3360	0.0038
12	4	9	12	3	10	5946.5173	0.0093
9	3	7	8	4	5	5962.4079	-0.0027
7	0	7	6	1	5	6104.0310	0.0018
9	1	9	8	2	7	6337.9098	-0.0003
13	6	7	12	7	6	6441.5113	-0.0052
14	4	11	14	3	12	6441.6075	0.0001
8	0	8	7	1	6	6645.5420	-0.0138
9	2	8	8	3	6	6779.6878	-0.0052
12	5	8	11	6	5	6780.3761	0.0004
15	4	12	15	3	13	6780.8011	0.0063
13	4	9	13	3	11	6841.4284	-0.0038
9	5	5	9	4	5	7058.0993	-0.0236
9	0	9	8	1	7	7126.8938	0.0139
10	3	8	9	4	6	7193.5801	-0.0111
10	0	10	9	1	8	7582.5488	-0.0078
5	3	2	5	0	5	7621.7694	-0.0059
10	2	9	9	3	7	7736.8441	-0.0007
14	6	9	13	7	6	7774.8546	0.0056
3	3	1	2	2	1	7827.6051	-0.0169

ľ	K'a	K'c	J″	K"a	К″с	Obs./MHz	Diff./MHz
1	1	1	0	0	0	2189.3643	-0.0032
2	1	2	1	0	1	3329.8025	-0.0038
3	1	3	2	0	2	4439.0266	-0.0020
4	1	4	3	0	3	5521.0384	-0.0029
5	1	5	4	0	4	6582.1601	-0.0036
6	1	6	5	0	5	7630.5315	-0.0133
3	0	3	2	1	2	2081.1440	0.0019
5	0	5	4	1	4	5235 9150	0.0015
6	0	6	5	1	5	6514,4494	-0.0001
7	0	7	6	1	6	7782.2122	-0.0045
2	2	1	1	1	0	5427.6616	0.0041
3	2	2	2	1	1	6568.0627	-0.0278
3	2	1	2	1	2	6778.0634	0.0021
4	2	3	3	1	2	7675.6660	-0.0067
5	1	5	4	2	2	2426.5207	0.0081
6	1	6	5	2	3	3361.8998	0.0053
7	1	7	6	2	4	4217.5961	0.0028
6	1	5	5	2	4	4821.7642	0.0043
8	1	8	6	2	5	4982.2423	0.0230
, ,	1	0 7	0	2	5	7626 0275	0.0110
7	2	6	6	2	3	3267 3308	-0.0214
7	2	5	6	3	4	3636 4063	-0.0072
8	2	7	7	3	4	4403.3025	-0.0117
8	2	6	7	3	5	4999.3425	0.0232
9	2	8	8	3	5	5504.5055	-0.0079
1	1	0	0	0	0	2254.2047	-0.0032
2	1	1	1	0	1	3524.3183	-0.0091
3	1	2	2	0	2	4827.9753	-0.0022
4	1	3	3	0	3	6168.7965	0.0021
5	1	4	4	0	4	7552.1723	-0.0047
3	0	3	2	1	1	2486.6213	-0.0002
4	0	4	3	1	2	3566.0319	-0.0115
5	0	5	4	1	3	4588.1479	-0.0125
ь 7	0	0 7	5	1	4	5544.4442	0.0080
8	0	8	7	1	6	7236 9878	-0.0022
9	0	9	8	1	7	7972.5331	-0.0070
2	2	1	1	1	1	5492.5072	0.0092
3	2	1	2	1	1	6583.5437	0.0035
3	2	2	2	1	2	6762.6310	0.0193
4	2	2	3	1	2	7721.6859	-0.0087
4	1	3	3	2	1	2071.8751	-0.0007
5	1	4	4	2	2	3396.5301	0.0043
5	1	4	4	2	3	3442.5663	0.0185
7	1	7	6	2	5	4424.9048	0.0031
0	1	5	5	2	3	4715.8101	0.0055
0 7	1	6	6	2	4	6013 9210	-0.0055
10	1	10	9	2	8	7068.2427	-0.0012
8	1	7	7	2	5	7274.6974	0.0163
6	2	4	5	3	2	2313.0946	-0.0037
7	2	6	6	3	4	3275.0742	-0.0014
7	2	5	6	3	3	3628.6744	-0.0156
8	2	7	7	3	5	4422.5033	0.0156
8	2	6	7	3	4	4980.1406	-0.0053
9	2	7	8	3	5	6363.6659	0.0038
10	2	8	9	3	6	7770.2043	-0.0074
8	3	5	/	4	5	2011.0245	-0.0054
9 10	3	8	o Q	4	5	5000 6542	-0.0103
7	1	6	7	-	7	2188 8734	0.0001
8	1	7	8	0	8	2590.6758	-0.0003
9	1	8	9	0	9	3055.7852	0.0038
10	1	9	10	0	10	3575.5153	-0.0003
11	1	10	11	0	11	4137.6497	0.0030
12	1	11	12	0	12	4728.2047	-0.0030
14	1	13	14	0	14	5942.0081	0.0029
8	2	6	8	1	7	2545.3357	-0.0118
7	2	5	7	1	6	2552.9781	-0.0054
9	2	7	9	1	8	2591.6249	-0.0017
ь	2	4	ь	1	5	2003.2423	-0.0151

Table S6: Line list for the fit obtained using the SPFIT program for *trans*-out-par, measured rotational transitions are shown as Obs. and the residuals are shown as Diff.

5	2	3	5	1	4	2682.8870	-0.0072
10	2	8	10	1	9	2701 0841	-0.0021
1	2	2	1	1	3	2777 38/9	-0.0058
2	2	1	2	1	2	2777.3043	0.0050
3	2	1	3	1	2	28/2.430/	0.0084
11	2	9	11	1	10	2881.2324	-0.0029
12	2	10	12	1	11	3137.7103	-0.0016
3	2	2	3	1	3	3245.8939	-0.0337
4	2	3	4	1	4	3379.1037	-0.0181
13	2	11	13	1	12	3473.5233	-0.0035
5	2	4	5	1	5	3546.9571	0.0047
6	2	5	6	1	6	3749.8563	-0.0029
14	2	12	1/	1	12	3887 0402	-0.0001
-14	2	12	7	1	- 13	2007.0024	-0.0001
/	2	0	/	1	/	3987.9834	0.0096
8	2	/	8	1	8	4260.9571	-0.0205
15	2	13	15	1	14	4375.6485	-0.0057
9	2	8	9	1	9	4568.0003	0.0048
10	2	9	10	1	10	4907.5373	-0.0080
11	2	10	11	1	11	5277.5525	0.0020
9	3	6	9	2	7	4556.6297	0.0095
8	3	5	8	2	6	4710 9369	-0.0017
7	2	1	7	2	5	4920 8702	-0.0024
, ,	2	4	, ,	2	J	4835.8753	-0.0034
6	3	3	6	2	4	4938.2396	0.0246
5	3	2	5	2	3	5005.9664	0.0027
4	3	1	4	2	2	5047.3750	0.0007
3	3	0	3	2	1	5069.0620	0.0025
3	3	1	3	2	2	5084.4143	-0.0022
4	3	2	4	2	3	5092.7476	-0.0007
5	3	3	5	2	4	5109 3356	0.0024
6	2	4	6	2	5	5127 8002	0.0002
7	2	-4 C	7	2	5	5157.8002	0.0003
,	2	5	,	2	7	5162.0258	-0.0255
8	3	6	8	2	/	5246.0087	-0.0279
10	3	8	10	2	9	5448.2114	0.0102
11	3	9	11	2	10	5592.8917	0.0183
13	3	11	13	2	12	5981.1866	-0.0133
12	4	8	12	3	9	6734.9709	0.0023
10	4	6	10	3	7	6947.3118	-0.0070
9	4	5	9	3	6	7010.4845	-0.0023
8	4	4	8	3	5	7052 6640	0.0037
7	4	3	7	3	1	7079 4728	0.0037
, o	4	5	, o	2	6	7092 2712	0.0050
0	4	2	6	2	2	7095.2715	0.0033
6	4	2	6	3	3	7095.5898	0.0028
11	4	8	11	3	9	/096.4505	-0.0054
7	4	4	7	3	5	7098.2438	-0.0066
6	4	3	6	3	4	7103.2147	0.0074
7	2	6	7	1	6	2191.6419	-0.0038
6	2	5	6	1	5	2395.9423	-0.0067
5	2	4	5	1	4	2576.9349	-0.0042
4	2	3	4	1	3	2731 3680	-0.0006
3	2	2	3	1	2	2856 9534	-0.0252
2	2	1	2	1	2	2050.5554	0.0232
5	2	2	3	1	5	3201.3803	0.0031
4	2	2	4	1	4	3425.1368	-0.0070
5	2	3	5	1	5	3652.9008	-0.0067
6	2	4	6	1	6	3957.1642	-0.0034
7	2	5	7	1	7	4349.3035	-0.0082
8	2	6	8	1	8	4837.8065	-0.0028
9	2	7	9	1	9	5427.1469	0.0026
10	2	8	10	1	10	6117.7449	0.0080
9	3	7	9	2	7	4474 4477	0.0066
0	2	6	ç	2	6	4660 1045	-0.0102
7	2	- -	7	2	5	4820 6822	0.0105
~	5	5		2	5	4820.0823	-0.0269
6	3	4	6	2	4	4930.4939	0.0024
5	3	3	5	2	3	5003.3852	0.0072
4	3	2	4	2	2	5046.7375	0.0112
3	3	1	3	2	1	5068.9635	-0.0033
3	3	0	3	2	2	5084.5110	0.0019
4	3	1	4	2	3	5093.3988	0.0025
5	3	2	5	2	4	5111.9226	0.0036
6	3	3	6	2	5	5145.5523	0.0289
7	2	1	7	2	6	5201 2230	0.0203
, o	5	-	, o	2	ט ד	5201.2230	0.0024
0	3	3	0	2	<i>'</i>	5267.7711	0.0008
9	5	ь _	9	2	ð	5415.7683	-0.0007
10	3	7	10	2	9	5597.5171	0.0036
15	4	12	15	3	12	6010.2819	-0.0057
13	4	10	13	3	10	6524.9225	-0.0102
11	4	8	11	3	8	6842.8511	0.0027
10	4	7	10	3	7	6940.5671	0.0139
9	4	6	9	3	6	7007.5635	-0.0035
		-	-	-	-		

8	4	5	8	3	5	7051.5358	0.0040
7	4	4	7	3	4	7079.0777	0.0007
9	4	5	9	3	7	7092.6711	0.0052
8	4	4	8	3	6	7094.3979	0.0038
6	4	3	6	3	3	7095.4898	0.0060
10	4	6	10	3	8	7096.6210	-0.0101
7	4	3	7	3	5	7098.6335	0.0055
6	4	2	6	3	4	7103.3138	0.0033
12	4	8	12	3	10	7141.3109	0.0199
5	4	2	5	3	2	7104.6830	-0.0051
5	4	1	5	3	2	7104.6830	-0.0258
5	4	2	5	3	3	7107.3002	0.0263
5	4	1	5	3	3	7107.3002	0.0057
4	4	1	4	3	1	7109.4685	0.0007
4	4	0	4	3	1	7109.4685	-0.0016
4	4	1	4	3	2	7110.1175	0.0017
4	4	0	4	3	2	7110.1175	-0.0006

6 2 5 3 3 2009 3349 0.0133 1 1 1 0 0 0 2196.5750 -0.0033 6 1 5 6 0 6 2210.6445 0.0041 2 0 2 1 0 1 2409.2468 -0.0075 7 1 6 7 0 7 2683.6220 -0.0065 7 1 6 7 0 7 2683.6220 -0.0065 4 2 2 4 1 3 2754.9949 0.0081 3 2 1 3 1 2928.5175 -0.0138 2 1 2 1 2 345.5020 -0.0299 3 1 3 2 1 2 3458.5202 -0.0299 3 1 3 32 2 2 1 377.8762 -0.0132 3 0	J'	K'a	K′c	J″	K"a	К"с	Obs./MHz	Diff./MHz
1 1 1 0 0 0 216.5750 -0.0033 6 1 5 6 0 6 2210.6445 0.0075 2 1 1 1 0 2210.7091 -0.0015 7 2 5 7 1 6 2584.0631 -0.0025 7 1 6 7 0 7 268.6220 -0.0032 3 0 3 2 1 2 2692.5781 -0.0081 3 2 1 3 1 2 2867.9798 -0.0081 3 2 1 2 1 2 316.9650 -0.0094 3 2 1 2 1 336.43227 -0.0055 4 0 4 3 1 2 3488.3123 -0.0064 4 2 3 4 1 4 3542.3413 0.00064 4 2 3 4 1 4 3542.3413 0.00055	6	2	5	5	3	3	2009.3349	0.0153
6 1 5 6 0 6 2210 0.0017 2 1 1 1 0 2409.2468 -0.0075 2 1 1 1 0 2501.7091 -0.0016 7 2 5 7 1 6 2501.7091 -0.0032 3 0 3 2 1 2 2683.6220 -0.0032 4 2 2 4 1 3 2754.9949 0.0081 3 2 1 3 1 22867.9798 -0.0035 2 2 0 2 1 1 2973.1235 0.0176 2 1 2 1 2 3228.5175 -0.0084 3 2 2 3 1 2 3458.5020 -0.0029 3 1 3 2 1 3577.8762 -0.0132 3 0 3 2 0 2 3602.2114 0.0118 3 1 2 2 1	1	1	1	0	0	0	2196.5750	-0.0033
2 0 2 1 0 1 2409.2468 -0.0075 2 1 1 1 0 2501.7091 -0.0065 7 1 6 7 0 7 2683.6220 -0.0025 3 0 3 2 1 2 2692.5781 -0.0065 4 2 2 4 1 3 2754.9949 -0.0035 2 0 2 1 1 2973.1235 -0.0176 2 2 0 2 1 2 3285.575 -0.0084 3 2 2 3 1 336.9550 -0.0094 3 2 2 3 1 2 3488.3123 -0.0066 4 2 3 4 1 4 3577.8762 -0.0132 3 1 2 3600.2982 -0.0065 -0.0073 3 1 2 3600.39479	6	1	5	6	0	6	2210.6445	0.0041
2 1 1 1 0 2501.7091 -0.0016 7 2 5 7 1 6 2584.0631 -0.0052 3 0 3 2 1 2 2692.5781 -0.0053 4 2 2 4 1 3 2754.9949 -0.0035 2 2 0 2 1 1 2973.1235 -0.0188 2 1 2 1 2 2867.9798 -0.0035 2 2 1 2 1 2 0.0055 4 0 1 3316.9650 -0.0094 3 2 2 3 1 3 3362.3227 -0.0055 4 3 1 2 3458.5020 -0.0209 3 1 3 3162.2114 -0.0132 3 0 3 2 0 2 3602.1144 -0.0132 3 1 2 2 1 37490.139 -0.0033 4<	2	0	2	1	0	1	2409.2468	-0.0075
7 2 5 7 1 6 7584.0631 -0.0065 7 1 6 7 0 7 2683.6220 -0.0065 4 2 2 4 1 3 2754.9949 0.0081 3 2 1 3 1 2 2692.5781 -0.0085 2 2 0 2 1 1 2973.1335 0.0176 2 2 0 2 1 1 2973.1325 -0.0084 3 2 2 3 1 3 3362.3227 0.0055 4 0 4 3 1 2 3488.5020 -0.0029 3 1 3 2 2 488.3123 -0.0064 4 2 3 4 1 4 3542.3413 0.0020 2 1 1 3778.762 -0.0132 3 3 2 2 1 3778.762 -0.0033 3 1 2 2 1 3778.762	2	1	1	1	1	0	2501.7091	-0.0016
7 1 6 7 2683.6220 -0.0032 3 0 3 2 1 2 2692.5781 -0.0065 4 2 2 4 1 3 2754.9949 0.0081 3 2 1 3 1 2 2867.9798 -0.0035 2 2 0 2 1 1 2973.1235 0.0176 2 2 1 2 1 2328.5175 -0.0188 3 2 2 3 1 3363.3227 0.0055 4 0 4 3 1 2 3488.3123 -0.0064 4 2 3 4 1 4 3542.3413 0.0020 2 1 1 1 0 1 3577.8762 -0.0132 3 2 2 2 1 3622.1114 0.0118 3 1 2 1 3622.1114 0.0118 3 1 3 3980.1340 -0.0024	7	2	5	7	1	6	2584.0631	-0.0065
3 0 3 2 1 2 262,5781 -0.0065 4 2 2 4 1 3 2754,9949 0.0081 3 2 1 3 1 22867,978 -0.0035 2 2 0 2 1 1 2973,1235 0.0176 2 2 1 2 1 2 3285,175 -0.0194 3 2 2 3 1 3 3366,3227 0.0055 4 0 4 3 1 2 3488,3123 -0.0064 4 2 3 4 1 4 3577,8762 -0.0132 3 0 3 2 0 2 3600,2982 -0.0065 3 1 2 1 1 3749,0139 -0.033 12 3 9 12 2 10 3936,8310 -0.0138 4 0	7	1	6	7	0	7	2683.6220	-0.0032
422413 2754.9949 0.0081 321312 2867.9798 -0.0035 220211 2973.1235 0.0176 221212 3228.5175 -0.0188 322313 3362.3227 0.0055 404312 3488.5020 -0.0209 313212 3488.3123 -0.0064 423414 3542.3413 0.0020 211101 3577.8762 -0.0132 303202 3600.2982 -0.00655 32221 3662.21144 0.0118 31221 3622.1144 0.0118 404313 3980.1340 -0.0024 625616 403.9255 -0.0040 734725 4769.3792 -0.0093 404313 3980.1340 -0.0026 633624 4921.2079 0.0063 414313 4778.679 -0.0026 633624 4921.2079 0.0003 414 <td>3</td> <td>0</td> <td>3</td> <td>2</td> <td>1</td> <td>2</td> <td>2692.5781</td> <td>-0.0065</td>	3	0	3	2	1	2	2692.5781	-0.0065
3 2 1 3 1 2 2867.9798 -0.0035 2 2 0 2 1 1 2973.1235 0.0176 2 2 1 2 1 2 3285.5175 -0.0188 2 1 2 1 0 1 3316.9650 -0.0094 3 2 2 3 1 2 3485.5020 -0.00209 3 1 3 2 1 2 3488.3123 -0.0064 4 2 3 4 1 4 3542.3413 0.0020 2 1 1 0 1 3577.8762 -0.0132 3 0 3 2 0 2 3600.2982 -0.0065 3 1 2 2 1 1 3749.0139 -0.0033 11 3 3 1 3 3801.340 -0.0024 6 2 5 6 1 6 4043.9255 -0.0043 11 4 <td>4</td> <td>2</td> <td>2</td> <td>4</td> <td>1</td> <td>3</td> <td>2754.9949</td> <td>0.0081</td>	4	2	2	4	1	3	2754.9949	0.0081
2 2 0 2 1 1 2973.1235 0.0176 2 1 2 1 2 3228.5175 -0.0084 3 2 2 3 1 3366.3227 0.0055 4 0 4 3 1 2 3458.5020 -0.0064 4 2 3 4 1 4 3542.3413 0.0020 2 1 1 1 0 1 3577.8762 -0.0033 3 2 2 2 1 3622.1114 0.0018 3 1 2 2 1 3749.0139 -0.0033 12 3 9 12 2 10 3986.1340 -0.0024 6 2 5 6 1 6 4043.9255 -0.0043 11 4 8 1 3 4443.202 -0.0043 14 4 3 1 3 4443.202 -0.0043 14 4 3 1 3 4451	3	2	1	3	1	2	2867.9798	-0.0035
2212123228.5175 -0.0188 2121013316.9650 -0.0094 3223123458.5020 -0.0209 3132123483.8123 -0.0064 423414542.3413 0.0020 2111013577.8762 -0.0132 3032023600.2982 -0.0065 3222213680.1340 -0.0033 1239122103936.8310 -0.0138 4043133980.1340 -0.0024 6256164043.9255 -0.0040 7347254769.3792 -0.0093 4043034775.8679 -0.0026 6336244921.2079 0.0063 414225102.0501 0.0011 4314225102.0511 0.0031 4311566.77594 0.0035 5054145268.0901 -0.0033 41422662.5767 0.0003 515644145268.7954 <td< td=""><td>2</td><td>2</td><td>0</td><td>2</td><td>1</td><td>1</td><td>2973.1235</td><td>0.0176</td></td<>	2	2	0	2	1	1	2973.1235	0.0176
2121013316.9650 -0.0094 3223133362.3227 0.0055 4043124358.5020 0.02209 3132123488.3123 0.0064 4234143542.3413 0.0020 21101357.8762 0.0132 3032023600.2982 0.0065 322213622.1114 0.0118 3122113749.0139 0.0033 1239122103936.8310 -0.0138 4043133980.1340 -0.0024 625616 643.3255 -0.0076 4143134645.1629 -0.00043 114810554134.4926 -0.0026 6336244921.2079 0.0003 414312491.7579 0.0003 4314225102.0501 0.0011 4314225102.0501 0.0003 5335244921.2079 0.0003 4143035	2	2	1	2	1	2	3228.5175	-0.0188
3 2 2 3 1 3 3362.3227 0.0055 4 0 4 3 1 2 3458.5020 -0.0029 3 1 3 2 1 2 3458.5020 -0.0032 4 2 3 4 1 4 3542.3413 0.0020 2 1 1 1 0 1 3577.8762 -0.0132 3 0 3 2 2 2 1 3622.1114 0.0118 3 1 2 2 1 1 3749.0139 -0.0033 12 3 9 12 2 10 3936.8310 -0.0024 6 2 5 6 1 6 4043.9255 -0.0040 7 3 4 7 2 5 4769.3792 -0.0026 6 3 3 6 2 4 4921.2079 0.0063 4 1 3 3 1 2 4991.7579 0.0003	2	1	2	1	0	1	3316.9650	-0.0094
4 0 4 3 1 2 3458.5020 -0.0209 3 1 3 2 1 2 3488.3123 -0.0064 4 2 3 4 1 4 3577.8762 -0.0132 3 0 3 2 0 2 3600.2982 -0.0065 3 2 2 2 1 37749.0139 -0.0033 12 3 9 12 2 10 3936.8310 -0.0148 3 1 2 2 1 3936.8310 -0.0024 6 2 5 6 1 6 404.32255 -0.0043 11 4 8 10 5 5 4134.4926 -0.0076 4 1 4 3 1 2 5 4763.9329 -0.00063 4 1 4 3 1 2 4991.7579 0.0063 4 1 3 1 2 2 5102.0501 0.0011 <td< td=""><td>3</td><td>2</td><td>2</td><td>3</td><td>1</td><td>3</td><td>3362.3227</td><td>0.0055</td></td<>	3	2	2	3	1	3	3362.3227	0.0055
3 1 3 2 1 2 348.3123 -0.0064 4 2 3 4 1 4 3542.3413 0.0020 2 1 1 0 1 357.78762 -0.0065 3 2 2 2 1 3662.1114 0.0132 3 0 3 2 2 1 1 3749.0139 -0.0033 12 3 9 12 2 10 3936.8310 -0.0138 4 0 4 3 1 3 3980.1340 -0.0024 6 2 5 6 1 6 4043.9255 -0.0043 11 4 8 10 5 5 4134.4926 -0.0076 4 1 4 3 1 3 4769.3792 -0.0026 6 3 3 6 2 4 4921.2079 0.0063 4 1 3 1 2 2 50.0001 0.0001 4	4	0	4	3	1	2	3458.5020	-0.0209
423414 3542.3413 0.0020 2111 3577.8762 -0.0132 303222 3600.2982 -0.0065 32221 3622.1114 0.0118 312211 3749.0139 -0.0033 123912210 3936.8310 -0.0024 625616 4043.9255 -0.0076 414313 465.1629 -0.0076 414303 4775.8679 -0.0026 633624 4921.2079 0.0063 404303 4775.8679 -0.0026 633624 4921.2079 0.0063 413312 4991.7579 0.0003 431422 5102.26011 0.0011 432423 5181.3878 -0.0021 634625 5259.2651 0.0021 505414 5797.5494 0.0033 414303 5440.8969 -0.0041 20111 5561.7954 0.0072 51541<	3	1	3	2	1	2	3488.3123	-0.0064
211101 3577.8762 -0.0132 303202 3600.2982 -0.0065 32221 3622.1114 0.0118 312211 3749.0139 -0.0033 123912210 3936.8310 -0.0138 404313 3980.1340 -0.0024 625616 403.9255 -0.0043 11481055 4134.4926 -0.0076 414313 4645.1629 -0.0040 734725 4769.3792 -0.0033 404303 4775.8679 -0.0026 633624 4921.2079 0.0063 413312 4991.7579 0.0003 431422 5181.3878 -0.0003 533524 5210.2540 -0.0021 634625 529.2651 0.0033 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 5561.7954 0.0072 5 <t< td=""><td>4</td><td>2</td><td>3</td><td>4</td><td>1</td><td>4</td><td>3542.3413</td><td>0.0020</td></t<>	4	2	3	4	1	4	3542.3413	0.0020
3 0 3 2 0 2 3600.2982 -0.0065 3 2 2 2 1 3622.1114 0.0118 3 1 2 2 1 1 3749.0139 -0.0033 12 3 9 12 2 10 3936.8310 -0.0138 4 0 4 3 1 3 3980.1340 -0.0024 6 2 5 6 1 6 4043.9255 -0.0043 11 4 8 10 5 5 4134.4926 -0.0040 7 3 4 7 2 5 4769.3792 -0.0093 4 0 4 3 0 3 4775.8679 -0.0036 4 1 3 3 1 2 4991.7579 0.0063 4 3 1 4 2 2 5102.0501 0.0011 4 3 1 4 2 3 518.13878 -0.0003 4 3 1 4 2 3 5102.0501 0.0021 6 3 4 6 2 5 5259.2651 0.0092 5 0 5 4 1 4 5268.0901 -0.0031 4 4 3 0 3 5440.8669 -0.0041 2 2 0 1 1 1 561.7954 0.0072 5 1 5	2	1	1	1	0	1	3577.8762	-0.0132
3 2 2 2 1 3622.1114 0.0118 3 1 2 2 1 1 3749.0139 -0.0033 12 3 9 12 2 10 3936.8310 -0.0024 6 2 5 6 1 6 4043.9255 -0.0043 11 4 8 10 5 5 4134.4926 -0.0076 4 1 4 3 1 3 4645.1629 -0.0040 7 3 4 7 2 5 4769.3792 -0.0093 4 0 4 3 0 3 4775.8679 -0.0026 6 3 3 6 2 4 4991.7579 0.0003 4 1 4 2 2 5102.0501 0.0011 4 3 2 4 2 2 5102.0501 0.0021 6 3 4 6 2 5 5259.2651 0.0092 5 3 3 52 4 5268.0901 -0.0033 4 1 4 3 0 3 5440.8969 -0.0041 2 2 0 1 1 1 5561.7954 0.0072 5 1 5 64 1 4 5797.5494 0.0035 5 2 4 2 3 6024.6275 -0.0008 5 2 4 2 2 <td>3</td> <td>0</td> <td>3</td> <td>2</td> <td>0</td> <td>2</td> <td>3600.2982</td> <td>-0.0065</td>	3	0	3	2	0	2	3600.2982	-0.0065
312211 3749.0139 -0.0033 123912210 3936.8310 -0.0138 404313 3980.1340 -0.0024 625616 4043.9255 -0.0043 11481055 4134.4926 -0.0076 414313 4645.1629 -0.0040 734725 4769.3792 -0.00266 633624 4921.2079 0.0063 413312 4991.7579 0.0003 431422 5102.0501 0.0011 432423 5181.3878 -0.0003 533524 5202.2240 -0.0021 634625 5259.2651 0.0072 505414 5797.5494 0.0035 505404 5933.1242 0.0004 523422 6850.6277 -0.0082 515 6945.0467 0.0093 66 51 5.67754 0.0072 515 6945.0467 0.0093 66 51 5.67754 0.0003 606 <td< td=""><td>3</td><td>2</td><td>2</td><td>2</td><td>2</td><td>1</td><td>3622.1114</td><td>0.0118</td></td<>	3	2	2	2	2	1	3622.1114	0.0118
123912210 3936.8310 -0.0138 404313 3980.1340 -0.0024 625616 4043.9255 -0.0043 11481055 4134.4926 -0.0076 414313 4645.1629 -0.0040 734725 4769.3792 -0.0093 404303 4775.8679 -0.0026 633624 4921.2079 0.0063 413312 4991.7579 0.0003 431422 5102.0501 0.0011 432423 5181.3878 -0.0021 533524 5210.2240 -0.0021 634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 5561.7554 0.0072 515404 5933.1242 0.0059 523422 6128.2394 0.0059 5156945.0467 0.0092 0.0014 65 <td>3</td> <td>1</td> <td>2</td> <td>2</td> <td>1</td> <td>1</td> <td>3749.0139</td> <td>-0.0033</td>	3	1	2	2	1	1	3749.0139	-0.0033
4043133980.1340 -0.0024 625616 4043.9255 -0.0043 11481055 4134.4926 -0.0076 414313 4645.1629 -0.0040 734725 4769.3792 -0.0093 404303 4775.8679 -0.0026 633624 4921.2079 0.0003 413312 4991.7579 0.0003 431422 5102.0501 0.0011 432423 5181.3878 -0.0021 634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 5561.7954 0.0072 515414 5797.5494 0.0035 523422 6128.2394 0.0059 515404 6425.5767 0.0003 606515 6945.0467 0.0092 616515 6945.0467 0.0092 6	12	3	9	12	2	10	3936.8310	-0.0138
625616 4043.9255 -0.0043 11481055 4134.4926 -0.0076 414313 4645.1629 -0.0040 734725 4769.3792 -0.0026 633624 4921.2079 0.0063 413312 4991.7579 0.0003 431422 5102.0501 0.0011 432423 5181.3878 -0.0003 533524 5210.2240 -0.0021 634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 561.7954 0.0072 515404 5933.1242 0.0004 523423 6024.6275 -0.0008 523422 612.82394 0.0059 515642.8750 0.0093 $32.2.2.2.1.1.1.6588.7195$ -0.0014 322211 6589.717 -0.0082 616515 6945.0467 0.0093 <td>4</td> <td>0</td> <td>4</td> <td>3</td> <td>1</td> <td>3</td> <td>3980.1340</td> <td>-0.0024</td>	4	0	4	3	1	3	3980.1340	-0.0024
114810554134.4926 -0.0076 4143134645.1629 -0.0040 7347254769.3792 -0.0093 4043034775.8679 -0.0026 6336244921.2079 0.0063 4133124991.7579 0.0003 4314225102.0501 0.0011 4324235181.3878 -0.0003 5335245210.2240 -0.0021 6346255259.2651 0.0092 5054145268.0901 -0.0033 4143035440.8969 -0.0041 2201115561.7954 0.0072 5154045933.1242 0.0004 523422 6128.2394 0.0059 5156404 6462.5767 0.0003 66515 6945.0467 0.0092 606515 6945.0467 0.0092 606515 6945.0467 0.00217 6165<	6	2	5	6	1	6	4043.9255	-0.0043
4143134645.1629 -0.0040 7347254769.3792 -0.0093 4043034775.8679 -0.0026 6336244921.2079 0.0063 4133124991.7579 0.0003 431422 5102.0501 0.0011 432423 5181.3878 -0.0003 533524 5210.2240 -0.0021 634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8869 -0.0041 220111 5561.7954 0.0072 515404 5933.1242 0.0004 523422 6128.2394 0.0059 515404 6462.5767 0.0003 606515 6542.8750 0.0093 322211 6589.7195 -0.0014 322211 6589.7195 -0.0014 322211 6589.7195 -0.0014 32 <td>11</td> <td>4</td> <td>8</td> <td>10</td> <td>5</td> <td>5</td> <td>4134.4926</td> <td>-0.0076</td>	11	4	8	10	5	5	4134.4926	-0.0076
734725 4769.3792 -0.0093 404303 4775.8679 -0.0026 633624 4921.2079 0.0063 413312 4991.7579 0.0003 431422 5102.0501 0.0011 432423 5181.3878 -0.0021 634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 5561.7954 0.0072 515404 5933.1242 0.0004 523423 6024.6275 -0.0008 515404 5933.1242 0.0059 515404 6462.5767 0.0003 606515 6945.0467 0.0093 322211 6589.7195 -0.0014 322212 6850.6277 -0.0082 616515 6945.0467 0.0093 32224 7219.5355 -0.0014 32	4	1	4	3	1	3	4645.1629	-0.0040
4043034775.8679 -0.0026 6336244921.20790.00634133124991.75790.00034314225102.05010.00114324235181.3878 -0.0003 5335245210.2240 -0.0021 6346255259.2651 0.0092 5054145268.0901 -0.0033 4143035440.8969 -0.0041 220111561.7954 0.0072 5154145797.5494 0.0035 523423 6024.6275 -0.0008 5154045933.1242 0.0059 5154046462.5767 0.0093 6065156542.8750 0.0033 322211 6589.7195 -0.0014 322212 6850.6277 -0.0082 616515 6945.0467 0.0093 32224 7219.5355 -0.0011 147113	7	3	4	7	2	5	4769.3792	-0.0093
6336244921.2079 0.0063 4133124991.7579 0.0003 431422 5102.0501 0.0011 432423 5181.3878 -0.0003 533524 5210.2240 -0.0021 634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 5561.7954 0.0072 515414 5797.5494 0.0035 505404 5933.1242 0.0004 523423 6024.6275 -0.0008 523422 6128.2394 0.0059 515404 6462.5767 0.0003 606515 6945.0467 0.0092 616515 6945.0467 0.00217 625524 7219.5355 -0.0101 634533 7268.5754 -0.0001 11471139 7284.3050 0.0076 6 <td< td=""><td>4</td><td>0</td><td>4</td><td>3</td><td>0</td><td>3</td><td>4775.8679</td><td>-0.0026</td></td<>	4	0	4	3	0	3	4775.8679	-0.0026
4133124991.7579 0.0003 431422 5102.0501 0.0011 432423 5181.3878 -0.0003 533524 5210.2240 -0.0021 634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 5561.7954 0.0072 515414 5797.5494 0.0035 505404 5933.1242 0.0004 523423 6024.6275 -0.00088 515404 6462.5767 0.0003 606515 6542.8750 0.0093 322211 6589.7195 -0.0014 322212 6850.6277 -0.0082 616505 7072.3400 0.0217 625524 7219.5355 -0.0101 1471139 7284.3050 0.0076 707616 7794.8844 0.0158 8<	6	3	3	6	2	4	4921.2079	0.0063
431422 5102.0501 0.0011 432423 5181.3878 -0.0003 533524 5210.2240 -0.0021 634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 5561.7954 0.0072 515404 5933.1242 0.0004 524423 6024.6275 -0.0008 523422 6128.2394 0.0059 515404 6462.5767 0.0003 606515 6542.8750 0.0093 322211 6589.7195 -0.0014 322212 6850.6277 -0.0082 616515 6945.0467 0.0092 66505 7072.3400 0.0217 625524 7193.5355 -0.0101 11471139 7284.3050 0.0018 615514 7454.9508 -0.0076 70 <td>4</td> <td>1</td> <td>3</td> <td>3</td> <td>1</td> <td>2</td> <td>4991.7579</td> <td>0.0003</td>	4	1	3	3	1	2	4991.7579	0.0003
432423 5181.3878 -0.0003 533524 5210.2240 -0.0021 634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 5561.7954 0.0072 515404 5933.1242 0.0004 524423 6024.6275 -0.0008 523422 6128.2394 0.0059 515404 6462.5767 0.0003 606515 6542.8750 0.0093 322211 6589.7195 -0.0014 322212 6850.6277 -0.0082 616515 6945.0467 0.0092 66505 7072.3400 0.0217 625524 719.5355 -0.0101 11471139 7284.3050 0.0108 615514 7454.9508 -0.0076 707616 7794.8844 0.0158 81 <td>4</td> <td>3</td> <td>1</td> <td>4</td> <td>2</td> <td>2</td> <td>5102.0501</td> <td>0.0011</td>	4	3	1	4	2	2	5102.0501	0.0011
533524 5210.2240 -0.0021 634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 561.7954 0.0072 515414 5797.5494 0.0035 505404 5933.1242 0.0004 524423 6024.6275 -0.0008 523422 6128.2394 0.0059 515404 6462.5767 0.0033 606515 6542.8750 0.0093 322211 6589.7195 -0.0014 322212 6850.6277 -0.0082 616515 6945.0467 0.0092 606505 7072.3400 0.0217 625514 7454.9508 -0.0001 11471139 7284.3050 0.0108 615514 7454.9508 -0.0076 707616 7794.8844 0.0158 8	4	3	2	4	2	3	5181.3878	-0.0003
634625 5259.2651 0.0092 505414 5268.0901 -0.0033 414303 5440.8969 -0.0041 220111 5561.7954 0.0072 515414 5797.5494 0.0035 505404 5933.1242 0.0004 523423 6024.6275 -0.0008 523422 6128.2394 0.0059 515404 6462.5767 0.0003 606515 6542.8750 0.0093 322211 6589.7195 -0.0014 322212 6850.6277 -0.0082 616505 7072.3400 0.0217 625524 7219.5355 -0.0101 11471139 7284.3050 0.0008 615514 7454.9508 -0.0076 707616 7794.8844 0.0158 817726 7895.3082 -0.0027	5	3	3	5	2	4	5210.2240	-0.0021
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	6	3	4	6	2	5	5259.2651	0.0092
414303 5440.8969 -0.0041 220111 5561.7954 0.0072 515414 5797.5494 0.0035 505404 5933.1242 0.0004 524423 6024.6275 -0.0008 523422 6128.2394 0.0059 515404 6462.5767 0.0003 606515 6542.8750 0.0093 322211 6589.7195 -0.0014 322212 6850.6277 -0.0082 616505 7072.3400 0.0217 625524 7219.5355 -0.0101 11471139 7284.3050 0.0108 615514 7454.9508 -0.0076 707616 7794.8844 0.0158 817726 789.3082 -0.0027	5	0	5	4	1	4	5268.0901	-0.0033
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	4	1	4	3	0	3	5440.8969	-0.0041
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2	2	0	1	1	1	5561.7954	0.0072
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5	1	5	4	1	4	5797.5494	0.0035
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5	0	5	4	0	4	5933.1242	0.0004
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5	2	4	4	2	3	6024.6275	-0.0008
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	2	3	4	2	2	6128.2394	0.0059
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	5	1	5	4	0	4	6462.5767	0.0003
3 2 2 2 1 1 6589.7195 -0.0014 3 2 2 2 1 2 6850.6277 -0.0082 6 1 6 5 1 5 6945.0467 0.0092 6 0 6 5 0 5 7072.3400 0.0217 6 2 5 5 2 4 7219.5355 -0.0101 6 3 4 5 3 3 7268.5754 -0.0001 11 4 7 11 3 9 7284.3050 0.0108 6 1 5 5 1 4 7454.9508 -0.0045 4 2 3 3 1 2 7665.8850 -0.0076 7 0 7 6 1 6 7794.8844 0.0158 8 1 7 7 2 6 7895.3082 -0.0027	6	0	6	5	1	5	6542.8750	0.0093
3 2 2 2 1 2 6850.6277 -0.0082 6 1 6 5 1 5 6945.0467 0.0092 6 0 6 5 0 5 7072.3400 0.0217 6 2 5 5 2 4 7219.5355 -0.0101 6 3 4 5 3 3 7268.5754 -0.0001 11 4 7 11 3 9 7284.3050 0.0108 6 1 5 5 1 4 7454.9508 -0.0045 4 2 3 3 1 2 7665.8850 -0.0076 7 0 7 6 1 6 7794.8844 0.0158 8 1 7 7 2 6 7895.3082 -0.0027	3	2	2	2	1	1	6589.7195	-0.0014
6 1 6 5 1 5 6945.0467 0.0092 6 0 6 5 0 5 7072.3400 0.0217 6 2 5 5 2 4 7219.5355 -0.0101 6 3 4 5 3 3 7268.5754 -0.0001 11 4 7 11 3 9 7284.3050 0.0108 6 1 5 5 1 4 7454.9508 -0.0045 4 2 3 3 1 2 7665.8850 -0.0076 7 0 7 6 1 6 7794.8844 0.0158 8 1 7 7 2 6 7895.3082 -0.0027	3	2	2	2	1	2	6850.6277	-0.0082
6 0 6 5 0 5 7072.3400 0.0217 6 2 5 5 2 4 7219.5355 -0.0101 6 3 4 5 3 3 7268.5754 -0.0001 11 4 7 11 3 9 7284.3050 0.0108 6 1 5 5 1 4 7454.9508 -0.0045 4 2 3 3 1 2 7665.8850 -0.0076 7 0 7 6 1 6 7794.8844 0.0158 8 1 7 7 2 6 7895.3082 -0.0027	6	1	6	5	1	5	6945.0467	0.0092
6 2 5 5 2 4 7219.5355 -0.0101 6 3 4 5 3 3 7268.5754 -0.0001 11 4 7 11 3 9 7284.3050 0.0108 6 1 5 5 1 4 7454.9508 -0.0045 4 2 3 3 1 2 7665.8850 -0.0076 7 0 7 6 1 6 7794.8844 0.0158 8 1 7 7 2 6 7895.3082 -0.0027	6	0	6	5	0	5	7072.3400	0.0217
6 3 4 5 3 3 7268.5754 -0.0001 11 4 7 11 3 9 7284.3050 0.0108 6 1 5 5 1 4 7454.9508 -0.0045 4 2 3 3 1 2 7665.8850 -0.0076 7 0 7 6 1 6 7794.8844 0.0158 8 1 7 7 2 6 7895.3082 -0.0027	6	2	5	5	2	4	7219.5355	-0.0101
11 4 7 11 3 9 7284.3050 0.0108 6 1 5 5 1 4 7454.9508 -0.0045 4 2 3 3 1 2 7665.8850 -0.0076 7 0 7 6 1 6 7794.8844 0.0158 8 1 7 7 2 6 7895.3082 -0.0027	6	3	4	5	3	3	7268.5754	-0.0001
6 1 5 5 1 4 7454.9508 -0.0045 4 2 3 3 1 2 7665.8850 -0.0076 7 0 7 6 1 6 7794.8844 0.0158 8 1 7 7 2 6 7895.3082 -0.0027	11	4	7	11	3	9	7284.3050	0.0108
4 2 3 3 1 2 7665.8850 -0.0076 7 0 7 6 1 6 7794.8844 0.0158 8 1 7 7 2 6 7895.3082 -0.0027	6	1	5	5	1	4	7454.9508	-0.0045
7 0 7 6 1 6 7794.8844 0.0158 8 1 7 7 2 6 7895.3082 -0.0027	4	2	3	3	1	2	7665.8850	-0.0076
8 1 7 7 2 6 7895.3082 -0.0027	7	0	7	6	1	6	7794.8844	0.0158
	8	1	7	7	2	6	7895.3082	-0.0027

 Table S7: Line list for the fit obtained using the SPFIT program for *cis*-out-par, measured rotational transitions are shown as Obs.

 and the residuals are shown as Diff.

 J' κ'_a κ'_c J'' κ''_a κ''_c Obs./MHz Diff./MHz

ľ	K'.	K'.	I"	K"-	K".	Obs./MHz	Diff./MHz
2	1	2	1	1	1	2521 4880	-0.0003
2	0	2	1	0	1	2600 2866	-0.0005
2	1	2	1	1	0	2003.2800	-0.0000
2	1	2	2	1	2	2776 2407	0.0011
2	1	2	2	1	2	2000 5647	-0.0096
3	0	3	2	0	2	3889.3047	0.0007
3	2	2	2	2	1	3928.9448	0.0015
3	2	1	2	2	0	3968.3349	0.0015
3	1	2	2	1	1	4069.0564	-0.0005
4	1	4	3	1	3	5024.7317	0.0070
4	0	4	3	0	3	5144.1700	-0.0040
4	2	3	3	2	2	5230.7728	0.0010
4	3	2	3	3	1	5256.8177	0.0056
4	3	1	3	3	0	5260.6573	0.0001
4	2	2	3	2	1	5325.1668	0.0033
4	1	3	3	1	2	5412.1362	0.0009
5	1	5	4	1	4	6266.0893	0.0002
5	0	5	4	0	4	6373.3585	0.0014
5	2	4	4	2	3	6525,9813	0.0052
5	3	3	4	3	2	6576 3642	-0.0113
5	3	2	4	3	1	6589 6385	0.0031
5	2	2	4	2	2	6700 5919	0.0052
5	1	1	4	1	2	6741 9071	0.0032
c	1	4	-	1	5	7500 2059	0.0021
0	1	0	5	1	5	7500.3958	0.0037
6	0	6	5	0	5	7584.5254	-0.0057
6	2	5	5	2	4	/813.0888	-0.0043
6	5	2	5	5	1	7882.9344	0.0153
6	5	1	5	5	0	7882.9344	-0.0013
6	4	3	5	4	2	7891.4890	0.0152
6	4	2	5	4	1	7892.6993	0.0006
6	3	4	5	3	3	7896.6880	-0.0088
6	3	3	5	3	2	7931.0826	-0.0047
5	4	2	4	4	1	6570.4677	0.0492
5	4	1	4	4	0	6570.6938	0.0010
1	1	0	0	0	0	2072.4207	-0.0038
2	1	1	1	0	1	3479.8919	0.0030
5	1	5	4	2	3	3619.0406	-0.0042
4	0	4	3	1	2	4094.0834	0.0039
2	2	0	1	1	0	4722.0060	0.0017
2	2	1	1	1	1	4809.8049	0.0033
3	1	2	2	0	2	4939,6630	0.0044
6	0	6	5	1	4	5897.9277	-0.0096
3	2	1	2	1	1	5973 2178	-0.0026
3	2	2	2	1	2	6217 2561	-0.0006
6	1	5	5	2	3	6276 9854	0.0059
1	1	3	3	0	3	6462 2136	-0.0162
- 0	1	0	0	2	7	7190 2916	-0.0001
3	2	2	2	2	2	7180.3810	-0.0001
4	2	2	3	1	2	7229.3200	-0.0072
3	3	0	2	2	0	7494.8055	0.0050
3	3	1	2	2	1	7504.2335	0.0009
7	1	6	6	2	4	7530.9585	-0.0035
9	2	8	8	3	6	/583.2/58	0.0038
4	2	3	3	1	3	7671.7730	0.0040
8	2	6	7	3	4	7815.5739	-0.0032
9	0	9	8	1	7	7880.2145	0.0000
3	2	1	3	1	3	2490.4014	-0.0032
4	2	2	4	1	4	2790.8510	0.0075
6	2	4	6	1	6	3810.1664	0.0020
9	3	7	9	2	7	2246.6253	0.0161
8	3	6	8	2	6	2589.7937	0.0062
7	3	5	7	2	5	2893.7987	0.0017
5	3	3	5	2	3	3333.3172	-0.0021
4	3	2	4	2	2	3457.5344	0.0039
3	3	0	3	2	2	3575,9359	0.0013
4	2	1	4	2	2	3605 8191	-0 0000
5	2	2	5	2	⊿	3669 4792	-0.0003
6	2	2	6	2	-+ 5	3787 4750	0.0001
7	2	 ∧	7	2	6	3986 0954	_0.0014
, o	2	+	2 2	2	7	1295 2765	_0 0021
0 10	5	כ ד	ن 10	2	7	4255.5705	-0.0031
010	4	/ E	0 TO	2	/ E	4230.0/44	-0.0210
0 7	4	c A	0 7	3	2	4/ 10.03/0	0.0037
, c	4	4	ć	3	4	4043.3200	-0.0029
0	4	5	ь -	3	3	491/.328/	0.0017
5	4	2	5	3	2	4956.9272	-0.0133

Table S8: Line list for the fit obtained using the SPFIT program for *trans*-out-perp conformer, measured rotational transitions are shown as Obs. and the residuals are shown as Diff.

6	4	2	6	3	4	4971.0070	0.0057
7	4	3	7	3	5	4974.9956	-0.0012
5	4	1	5	3	3	4974.9956	-0.0039
4	4	0	4	3	2	4980.6856	0.0035
8	4	4	8	3	6	4997.6152	-0.0036
9	4	5	9	3	7	5054.7152	0.0023
9	5	5	9	4	5	6304.0903	-0.0015
11	5	6	11	4	8	6319.9556	0.0083
10	5	5	10	4	7	6329.5118	-0.0028
9	5	4	9	4	6	6347.3420	-0.0014
7	5	3	7	4	3	6377.3542	0.0007
7	5	2	7	4	4	6383.0241	-0.0004
6	5	2	6	4	2	6394.0678	-0.0051
6	5	1	6	4	3	6395.6363	0.0115

ľ	K'a	K′c	J″	K"a	К"с	Obs./MHz	Diff./MHz
2	1	2	1	1	1	2516.1147	-0.0044
2	1	1	1	1	0	2699.9533	0.0022
3	1	3	2	1	2	3768.9532	-0.0025
3	0	3	2	0	2	3877.6416	0.0030
3	2	2	2	2	1	3912.0408	-0.0031
3	2	1	2	2	0	3946.4622	0.0051
3	1	2	2	1	1	4044.1924	0.0098
4	1	4	3	1	3	5016.2256	0.0018
4	0	4	3	0	3	5133.1169	-0.0014
4	2	3	3	2	2	5209.2453	-0.0019
4	3	2	3	3	1	5232.0558	0.0105
4	3	1	3	3	0	5235.1528	-0.0012
4	2	2	3	2	1	5292.1685	0.0015
4	1	3	3	1	2	5380.7841	0.0048
5	1	5	4	1	4	6257.1285	-0.0083
5	0	5	4	0	4	6365.0753	-0.0016
5	2	4	4	2	3	6500.6809	0.0104
5	3	3	4	3	2	6544.9634	-0.0011
5	2	3	4	2	2	6655.4599	0.0003
5	1	4	4	1	3	6705.9626	-0.0098
6	1	6	5	1	5	7491.6175	0.0046
6	0	6	5	0	5	7579.1450	-0.0105
6	2	5	5	2	4	7785.0139	-0.0001
6	3	4	5	3	3	7858.8274	-0.0032
6	3	3	5	3	2	7886.7971	-0.0118
2	1	2	1	0	1	3193.6974	-0.0066
6	1	6	5	2	3	4322.6203	0.0058
3	1	3	2	0	2	4363.3506	-0.0039
4	0	4	3	1	3	4647.4025	0.0002
2	2	1	1	1	0	4732.6911	-0.0118
2	2	0	1	1	1	4833.3504	0.0003
4	1	4	3	0	3	5501.9385	-0.0012
3	2	2	2	1	1	5944.7773	-0.0183
5	0	5	4	1	4	5996.2588	0.0034
3	2	1	2	1	2	6263.6973	0.0092
6	1	5	5	2	4	6491.3420	0.0018
5	1	5	4	0	4	6625.9502	-0.0080
6	0	6	5	1	5	7318.2857	0.0115
3	3	1	2	2	0	7526.2357	0.0002
3	3	0	2	2	1	7535.4809	-0.0070
6	1	6	5	0	5	7752.4963	0.0020
4	2	2	3	1	3	7786.9203	0.0209
8	2	6	8	1	7	2117.4890	0.0045
5	2	4	5	1	5	2888.1504	0.0053
6	2	5	6	1	6	3181.5453	-0.0009
4	3	2	4	2	3	3645.7207	-0.0003
5	3	3	5	2	4	3690.0227	0.0078
7	3	5	7	2	6	3874.6779	0.0053
8	3	6	8	2	7	4028.8016	-0.0068
9	3	7	9	2	8	4230.7246	-0.0035
11	4	7	11	3	8	4270.5167	-0.0017
9	4	5	9	3	6	4696.0281	0.0187
8	4	4	8	3	5	4841.4936	0.0078
7	4	4	7	3	5	5037.6626	-0.0110
6	4	3	6	3	4	5039.3845	0.0120
8	4	4	8	3	6	5057.5554	0.0026
9	4	6	9	3	7	5069.0534	-0.0210
7	6	1	7	5	2	7931.6898	-0.0166
7	6	2	7	5	3	7931.7961	0.0149

 Table S9: Line list for the fit obtained using the SPFIT program for *cis*-out-perp conformer, measured rotational transitions are shown as Obs. and the residuals are shown as Diff.

 J'
 K'_a K'_c J"
 K''_a K''_c Obs./MHz

01101111	0 0 0001 0111							
J	K'a	K′c	J‴	K"a	К"с	Symm.	Obs./MHz	Diff./MHz
1	1	0	0	0	0	А	2019.8957	-0.0009
1	1	0	0	0	0	F	2019 8957	-0.0006
I C	2	0	0	0	5	L	2013.8337	-0.0000
6	2	6	6	1	5	A	2022.5574	0.0003
6	2	6	6	1	5	E	2022.5574	0.0007
4	2	4	4	1	3	Α	2035.1088	0.0002
4	2	4	4	1	3	E	2035,1088	-0.0005
2	-			-	2	_	2000.2000	0.0054
3	Z	3	3	1	2	A	2077.8513	-0.0054
3	2	3	3	1	2	E	2077.8513	-0.0063
4	1	3	3	2	1	Α	2078.2844	-0.0013
4	1	3	3	2	1	F	2078 2844	-0.0010
1	1	0	0	-	-	_	2070.2011	0.0017
1	1	0	0	0	0	A	2120.7401	-0.0017
1	1	0	0	0	0	E	2128.7481	-0.0012
3	2	3	3	1	2	A	2132.5369	0.0043
3	2	3	3	1	2	E	2132.5369	0.0034
7	2	7	7	1	6	۵	2162 6566	-0.0002
,	2	,	,	1	0	-	2102.0500	0.0002
/	2	/	/	1	6	E	2162.6566	0.0015
6	3	5	5	4	2	A	2183.6638	0.0065
6	3	5	5	4	2	E	2183.7072	-0.0051
2	2	2	2	1	1	۸	2244 0148	0.0067
2	2	2	2	1	1	-	2244.0140	0.0007
2	2	2	2	1	1	E	2244.9148	0.0057
5	2	4	4	3	1	A	2316.2274	-0.0016
5	2	4	4	3	1	E	2316.2274	0.0034
6	1	6	6	0	6	۸	2401 2642	-0.0030
0	1	0	0	0	0	Ä	2401.2043	-0.0030
6	1	6	6	0	6	E	2401.2643	0.0017
8	2	8	8	1	7	A	2426.0314	-0.0003
8	2	8	8	1	7	E	2426.0314	0.0032
2	1	1	1	1	1	Δ	2441 7165	-0.0024
2	1	1	1	1	1	-	2441.7105	0.0024
2	1	1	1	T	1	E	2441.7165	-0.0018
2	0	1	1	0	1	A	2539.4933	0.0038
2	0	1	1	0	1	E	2539.4933	0.0047
2	1	1	1	1	0	Δ	2659 4259	0.0006
2	1	1	1	1	0	- -	2055.4255	0.0000
2	1	1	1	1	0	E	2059.4259	0.0018
5	2	4	4	3	2	A	2673.8168	0.0010
5	2	4	4	3	2	E	2673.8168	0.0023
3	2	3	3	1	3	Α	2730.2669	0.0014
2	2	2	2	1	2	E	2720 2660	0.0022
2	2	2	3	1	3	L	2730.2009	0.0022
3	0	2	2	1	1	A	2808.8588	-0.0063
3	0	2	2	1	1	E	2808.8588	-0.0055
9	2	9	9	1	8	Α	2822.6073	-0.0031
9	2	9	9	1	8	F	2822 6073	0.0025
5	2	5	5	2	6	L .	2022.0075	0.0023
8	3	8	ð	2	Ь	A	2907.6618	0.0042
8	3	8	8	2	6	E	2907.6618	-0.0002
5	1	4	4	2	2	Α	2943.9093	-0.0045
5	1	4	4	2	2	F	2943 9093	-0.0053
4	-			-	_	_	2050 5125	0.0015
4	Z	4	4	1	4	A	2959.5135	-0.0015
4	2	4	4	1	4	E	2959.5135	-0.0001
7	1	7	7	0	7	A	3015.2416	-0.0059
7	1	7	7	0	7	E	3015.2416	0.0003
10	3	10	10	2	8	۵	3018 0/17	-0.0060
10	5	10	10	2	0	-	3010.0417	0.0000
10	3	10	10	2	8	E	3018.0417	-0.0063
9	3	9	9	2	7	A	3061.8296	0.0109
9	3	9	9	2	7	E	3061.8296	0.0093
11	3	11	11	2	9	Δ	3095 9666	-0.0132
11	2	11	11	2	0	5	2005.0000	0.0132
11	3	11	11	Z	9	E	3095.9000	-0.0113
4	2	4	4	1	4	A	3118.6952	-0.0033
4	2	4	4	1	4	E	3118.6952	-0.0011
8	4	7	7	5	2	Δ	3130 0999	-0.0013
0	4	7	7	5	2	E	2120.0510	0.0027
0	4	/	/	5	2	E	5129.9510	-0.0037
3	0	2	2	1	2	A	3135.4230	-0.0018
3	0	2	2	1	2	E	3135.4230	-0.0002
8	4	7	7	5	3	А	3148.1828	0.0104
8	4	7	7	5	2	F	3148 3097	0 0006
5	+	,	,	5	ر م	L .	31-0.3037	0.0000
4	1	3	3	2	1	A	3161.8/23	-0.0032
4	1	3	3	2	1	E	3161.8723	-0.0001
2	1	1	1	0	1	А	3186.3268	-0.0011
2	1	1	1	0	-	F	3186 3268	-0.0006
<u>_</u>	-	- -	- -	5	1	L .	3100.3200	0.0000
ð	3	ŏ	ŏ	2	ь	A	3190.9323	-0.0009
8	3	8	8	2	6	E	3196.9323	-0.0032
4	1	3	3	2	2	Α	3216.5496	-0.0018
4	1	3	3	2	2	F	3216 5496	0.0014
-	2	7	7	2	-	~	2246 7720	0.001-7
<u>/</u>	3	/	/	2	5	A _	3245.//20	0.0047
7	3	7	7	2	5	E	3245.7720	0.0014
5	2	5	5	1	5	А	3248.6737	-0.0021

Table S10: Line list for the fit obtained using the XIAM program for *cis*-in-perp conformer, measured rotational transitions areshown as Obs. and the residuals are shown as Diff.J'K'aK'cJ'K''aK''aK''aJ'K'aK'cJ'Symm.Obs./MHzDiff./MHz

F	2	-	-	1	-	-	2248 6727	0.0001
5	2	5	5	1	5	E .	3248.0737	0.0001
12	3	12	12	2	10	A	3316.2248	0.0045
12	3	12	12	2	10	E	3316.2248	0.0090
10	2	10	10	1	9	A	3349.6321	0.0018
10	2	10	10	1	9	E	3349.6321	0.0097
7	3	7	7	2	5	А	3384.3888	0.0020
7	3	7	7	2	5	E	3384.3888	-0.0004
7	3	6	6	4	2	Α	3416 2827	0.0156
7	3	6	6	4	2	F	3/16 2373	-0.0120
6	2	5	5		2	L ^	2406 1690	0.0120
0	2	5	5	3	2	A	3490.1089	-0.0031
6	2	5	5	3	2	E	3496.1689	-0.0002
2	1	1	1	0	1	A	3512.8864	-0.0012
2	1	1	1	0	1	E	3512.8864	0.0001
6	3	6	6	2	4	A	3524.5965	-0.0045
6	3	6	6	2	4	E	3524.5965	-0.0068
7	3	6	6	4	3	А	3556.5810	0.0169
7	3	6	6	4	3	E	3556.5810	0.0082
6	3	6	6	2	4	Α	3581 9832	0.0005
6	3	6	6	2	1	F	3581 9832	-0.0017
6	3	6	6	2	4	L ^	2505.202	-0.0017
0	2	0	0	1	0	A F	3590.0371	-0.0010
6	2	6	6	1	Б	E	3596.6371	0.0022
6	1	5	5	2	3	A	3652.8250	-0.0053
6	1	5	5	2	3	E	3652.8250	-0.0077
3	1	2	2	1	2	A	3655.9648	-0.0014
3	1	2	2	1	2	E	3655.9648	-0.0005
13	3	13	13	2	11	А	3689.1646	-0.0103
13	3	13	13	2	11	E	3689,1646	-0.0026
8	1	8	8	0	8	Δ	3691 5783	-0.0031
0	1	0	0	0	0	F	2601 5782	0.0031
о г	2	5	5	2	2	L ^	2752 2022	0.0040
5	2	5	5	2	2		3753.2352	-0.0031
5	3	5	5	2	3	E	3/53.2932	-0.0052
3	0	2	2	0	2	A	3/82.26/9	0.0047
3	0	2	2	0	2	E	3782.2679	0.0059
3	2	2	2	2	1	A	3825.8417	-0.0061
3	2	2	2	2	1	E	3825.8417	-0.0051
3	2	2	2	2	0	Α	3869.4402	0.0003
3	2	2	2	2	0	E	3869.4402	0.0023
4	3	4	4	2	2	Δ	3871 4203	-0.0005
1	3	4	4	2	2	F	3871 /203	0.0003
4	2	4	4	2	2	L ^	3871.4203	0.0012
4	5	4	4	2	2	A .	3870.3020	0.0014
4	3	4	4	2	2	E	38/6.3620	-0.0022
3	3	3	3	2	1	A	3947.8279	0.0188
3	3	3	3	2	1	E	3947.8279	0.0003
3	1	2	2	1	1	A	3981.8129	-0.0024
3	1	2	2	1	1	E	3981.8129	-0.0007
11	2	11	11	1	10	А	3987.9264	-0.0153
11	2	11	11	1	10	E	3987.9264	-0.0052
14	4	14	14	3	11	А	3996.7294	0.0006
14	4	14	14	3	11	F	3996 7294	-0.0011
7	2	7	7	1	7	^	4000 1542	-0.0011
7	2	7	7	1	7		4000.1542	-0.0018
/	2	/	/	1	/	E	4000.1542	0.0026
3	3	3	3	2	2	A	4001.7632	-0.0119
3	3	3	3	2	2	E	4001.7632	0.0057
3	3	3	3	2	2	A	4002.5037	0.0187
3	3	3	3	2	2	E	4002.5037	0.0002
6	1	5	5	2	4	А	4005.4751	-0.0024
6	1	5	5	2	4	E	4005.4751	-0.0031
15	4	15	15	3	12	Α	4006 6981	0.0028
15	1	15	15	3	12	F	4006 6981	0.0040
15	7	15	15	2	2	L ^	4000.0001	0.0040
4	5	4	4	2	5	A .	4030.0033	-0.0008
4	3	4	4	2	3	E	4030.6035	0.0016
4	3	4	4	2	3	A	4035.5515	0.0074
4	3	4	4	2	3	E	4035.5515	0.0046
5	3	5	5	2	4	A	4086.4105	-0.0034
5	3	5	5	2	4	E	4086.4105	-0.0026
5	3	5	5	2	4	А	4105.9442	0.0008
5	3	5	5	2	4	E	4105.9442	0.0004
13	4	13	13	3	10	А	4119.2966	0,0098
13	1	13	13	2	10	F	4119 2966	0.0050
10		<u>د</u>	0	5	2	~	A100 0400	.0 0021
10	- -	9	9	c	ر ۸	~	4127 400F	0.0021
10	5	Э	Э	o c	4	A -	4127.4985	-0.0021
10	5	9	9	6	4	E .	412/./132	0.0012
6	2	5	5	3	2	A	4150.5877	-0.0055
6	2	5	5	3	2	E	4150.5877	0.0004
6	2	5	5	3	3	Α	4170.1252	0.0024
6	2	5	5	3	3	E	4170.1252	0.0072
6	3	6	6	2	5	А	4179.0181	-0.0041

6	2	6	c	2	E	-	4170 0191	0 0022
-	5	0	0	2	5	E .	41/9.0101	-0.0035
/	1	6	6	2	4	A	4187.5877	-0.0035
7	1	6	6	2	4	E	4187.5877	-0.0081
14	3	14	14	2	12	A	4212.0998	-0.0020
14	3	14	14	2	12	E	4212.0998	0.0090
6	3	6	6	2	5	Α	4236.3966	-0.0073
6	3	6	6	2	5	E	4236.3966	-0.0065
6	2	6	6	1	6	А	4251.0537	-0.0055
6	2	6	6	1	6	E	4251.0537	0.0007
3	1	2	2	0	2	А	4302.8006	-0.0040
3	1	2	2	0 0	2	F	4302 8006	-0.0035
7	2	7	7	2	6	~	4302.0000	0.0055
7	5	7	7	2	0	A F	4317.3901	0.0017
/	3	/	/	2	6	E	4317.3961	0.0031
12	4	12	12	3	9	A	4337.6892	0.0045
12	4	12	12	3	9	E	4337.6892	-0.0003
9	1	9	9	0	9	A	4396.2484	-0.0070
9	1	9	9	0	9	E	4396.2484	0.0004
11	4	11	11	3	8	A	4397.0539	0.0026
11	4	11	11	3	8	E	4397.0539	-0.0041
9	4	8	8	5	3	Α	4445.8197	-0.0024
9	4	8	8	5	3	Е	4445.7475	-0.0054
8	2	8	8	1	8	Δ	4453 8230	-0.0016
8	2	8	8	- 1	8	F	1153 8230	0.0044
7	2	7	7	2	6	L	4455.0250	0.0074
7	5	7	7	2	0	A F	4450.0175	0.0050
	3	/	/	2	0	Ē	4450.0175	0.0058
4	0	3	3	1	3	A	4476.0424	-0.0025
4	0	3	3	1	3	E	4476.0424	-0.0005
9	4	8	8	5	4	A	4491.8784	-0.0124
9	4	8	8	5	4	E	4491.9336	-0.0149
8	3	8	8	2	7	А	4508.7517	0.0000
8	3	8	8	2	7	E	4508.7517	0.0021
8	1	7	7	2	5	А	4545.5989	0.0078
8	1	7	7	2	5	F	4545 5989	0.0002
5	1	1	1	2	2	<u> </u>	4557 1749	0.0007
5	1	4	4	2	2		4557 1745	0.0007
7	2	4	4	2	2	L	4557.1745	0.0042
-	2	0	6	3	3	A	4605.7629	-0.0015
	2	6	6	3	3	E	4605.7629	0.0005
11	4	11	11	3	8	A	4606.6703	0.0068
11	4	11	11	3	8	E	4606.6703	0.0019
8	3	7	7	4	3	A	4693.9085	0.0024
8	3	7	7	4	3	E	4693.9085	0.0105
8	3	7	7	4	4	Α	4699.9884	-0.0017
8	3	7	7	4	4	E	4699.9884	-0.0011
11	1	10	10	2	8	Α	4701.1428	0.0212
11	1	10	10	2	8	E	4701.1428	-0.0022
12	2	12	12	1	11	А	4704.4351	-0.0035
12	2	12	12	1	11	F	4704 4351	0.0082
5	0	1	1	- 1	3	<u> </u>	1711 8573	-0.0073
5	0	4	4	1	3	F	4711.0573	-0.0078
5	1	4	4	2	2	L	4716 2595	0.0070
5	1	4	4	2	2		4710.3383	0.0003
5	1	4	4	2	3	E	4/16.3585	0.0051
9	1	8	8	2	6	A	4/36.8302	0.0147
9	1	8	8	2	6	E	4/36.8302	0.0035
9	3	9	9	2	8	A	4757.9047	-0.0012
9	3	9	9	2	8	E	4757.9047	0.0020
8	3	8	8	2	7	Α	4798.0216	-0.0058
8	3	8	8	2	7	E	4798.0216	-0.0016
7	1	6	6	2	5	Α	4842.0117	-0.0007
7	1	6	6	2	5	Е	4842.0117	-0.0024
4	1	3	3	1	3	Δ	4863 2261	-0.0011
1	1	3	3	- 1	3	F	4863 2261	0,0000
4 1E	2	15	15	2	12	L ^	4003.2201	0.0000
15	5	15	15	2	13	A F	4005.0170	-0.0055
15	5	13	13	2	15	E .	4003.0170	0.0088
10	4	10	10	3	/	A	48/9.825/	-0.0005
10	4	10	10	3	7	E	4879.8257	-0.0049
2	2	1	1	1	0	A	4893.2482	-0.0013
2	2	1	1	1	0	E	4893.2482	-0.0002
2	2	1	1	1	0	А	4904.3426	0.0093
2	2	1	1	1	0	E	4904.3426	0.0094
19	5	19	19	4	15	А	4911.3012	0.0073
19	5	19	19	4	15	E	4911.3012	0.0071
9	2	9	9	1	9	А	4950.5300	-0.0043
9	2	q	q	- 1	9	F	4950 5300	0.0045
3	<u>د</u> 1	2	2	0	2	<u>_</u>	1925 2028	
Э	1	2	2	0	2	A F	4333.2038	-0.0095
3	1	2	2	U	2	E .	4955.2038	-0.0074
18	5	18	18	4	14	A	49/4.6658	0.0031
18	5	18	18	4	14	E	4974.6658	-0.0011

0	2	7	7	4	4	•	1080 2646	0.0012
0	3	/	/	4	4	A	4989.2040	-0.0012
8	3	/	/	4	4	E	4989.2646	0.0014
4	0	3	3	0	3	A	4996.5749	-0.0114
4	0	3	3	0	3	E	4996.5749	-0.0100
2	2	1	1	1	1	A	5013.1965	0.0099
2	2	1	1	1	1	E	5013.1965	0.0102
10	3	10	10	2	9	А	5066.8451	0.0036
10	3	10	10	2	9	E	5066.8451	0.0080
9	4	9	9	3	6	Δ	5073 8270	0.0076
0	4	0	0	2	6	5	5073.0270	0.0070
9	4	9	9	5	0	E	5073.8270	0.0044
4	2	3	3	2	2	A	5092.4746	-0.0020
4	2	3	3	2	2	E	5092.4746	-0.0003
10	1	10	10	0	10	A	5101.6937	-0.0015
10	1	10	10	0	10	E	5101.6937	0.0049
12	6	11	11	7	4	A	5110.7185	-0.0028
12	6	11	11	7	4	E	5110.4058	-0.0124
12	6	11	11	7	5	А	5112.1809	0.0021
12	6	11	11	7	5	F	5112 4577	-0.0092
0	4	0	0	2	6	_	5110 2660	-0.0121
0	4	9	9	2	6	5	E110 2660	-0.0121
9	4	9	9	5	0	E	5119.5009	-0.0137
4	3	3	3	3	1	A	5121.3132	0.0074
4	3	3	3	3	1	E	5121.3132	-0.0061
4	3	3	3	3	0	A	5125.5311	-0.0046
4	3	3	3	3	0	E	5125.5311	0.0128
17	5	17	17	4	13	A	5177.0016	-0.0017
17	5	17	17	4	13	E	5177.0016	-0.0084
4	2	3	3	2	1	А	5196,9813	-0.0029
4	2	3	3	2	1	F	5196 9813	-0.0005
	4	2	8	2	5	~	5285 0112	-0.0003
0	4	0	0	2	5	5	5205.9115 E20E 0112	-0.0007
0	4	0	0	2	5	L	5285.5115	-0.0018
9	3	9	9	2	8	A	5294.1543	-0.0265
9	3	9	9	2	8	E	5294.1543	-0.0196
4	1	3	3	1	2	A	5294.4069	-0.0013
4	1	3	3	1	2	E	5294.4069	0.0010
8	4	8	8	3	5	A	5303.8702	0.0053
8	4	8	8	3	5	E	5303.8702	0.0018
4	1	3	3	0	3	А	5383.7664	-0.0021
4	1	3	3	0	3	E	5383,7664	-0.0017
7	4	7	7	3	4	Δ	5429 8799	0.0053
7		7	7	2		F	5/20 8700	0.0001
11	4	11	11	2	4	L	5425.0755	0.0001
11	3	11	11	2	10	A	5434.5713	-0.0018
11	3	11	11	2	10	E	5434.5713	0.0041
11	5	10	10	6	4	A	5446.5551	-0.0099
11	5	10	10	6	5	A	5460.3647	0.0228
13	2	13	13	1	12	A	5460.3647	0.0129
13	2	13	13	1	12	E	5460.3647	0.0256
6	0	5	5	1	4	А	5468.1349	0.0072
6	0	5	5	1	4	E	5468.1349	0.0055
16	5	16	16	4	12	Δ	5475 2214	-0.0037
16	5	16	16	4	12	F	5475 2214	-0.0116
10	2	10	10	4	12	L	5475.2214	-0.0110
10	2	10	10	1	10	A	5482.2591	-0.0047
10	2	10	10	1	10	E	5482.2591	0.0063
6	4	6	6	3	3	A	5506.8924	0.0006
6	4	6	6	3	3	E	5506.8924	-0.0139
5	4	5	5	3	2	E	5548.8573	-0.0027
5	4	5	5	3	2	А	5549.2692	0.0128
5	4	5	5	3	2	Е	5549.3131	-0.0021
7	4	7	7	3	5	А	5562 4151	0.0051
7	1	7	7	3	5	F	5562 /151	0.0083
6	4	, c	, c	2	1	L A	5502.4151	0.0003
0	4	0	0	5	4	A .	5502.5949	-0.0011
6	4	6	6	3	4	E	5562.5949	0.0118
5	4	5	5	3	3	A	5568.4415	-0.0067
5	4	5	5	3	3	E	5568.3934	0.0028
4	4	4	4	3	1	A	5570.1620	-0.0007
4	4	4	4	3	1	E	5570.2912	-0.0046
4	4	4	4	3	2	А	5575.0611	-0.0037
4	4	4	4	3	2	E	5574.9287	-0.0041
8	4	8	8	3	6	А	5575.1952	0.0076
8	4	8	8	3	6	E	5575 1952	0.0085
8	4	8	R	2	6	Δ	5593 1513	0.0000
0	4	0	0	2	6	Ē	5502 1513	0.0100
0	4	0	0	с С	7	E ^	5535.1313	0.0093
Э	4	9	9	3	/	A	5010.0911	-0.0032
9	4	9	9	3	/	E	5610.0911	-0.0027
8	2	7	7	3	4	A	5615.0282	-0.0007
8	2	7	7	3	4	E	5615.0282	0.0001
16	3	16	16	2	14	А	5615.8259	-0.0295
16	3	16	16	2	14	E	5615.8259	-0.0129

•	1	7	7	2	c	•	5617 2170	0.0004
0	1	/	/	2	0	A	5617.2178	-0.0004
8	1	/	/	2	6	E	5617.2178	-0.0033
10	4	10	10	3	8	A	5677.2291	0.0001
10	4	10	10	3	8	E	5677.2291	0.0010
7	2	6	6	3	3	A	5677.3940	0.0024
7	2	6	6	3	3	E	5677.3940	0.0091
7	2	6	6	3	4	А	5734.7742	0.0009
7	2	6	6	3	4	F	5734 7742	0.0075
10	1	Q	G G	5		Δ	5765 3921	0.0192
10	4	0	0	5	4	5	E76E 2414	0.0152
10	4	9	9	5	4	E	5705.3414	-0.0050
11	4	11	11	3	9	A	5786.4978	0.0009
11	4	11	11	3	9	E	5786.4978	0.0024
11	1	11	11	0	11	A	5792.1974	0.0045
11	1	11	11	0	11	E	5792.1974	0.0074
5	0	4	4	1	4	A	5795.4563	0.0019
5	0	4	4	1	4	E	5795.4563	0.0042
15	5	15	15	4	11	Α	5818.6865	-0.0058
15	5	15	15	4	11	E	5818.6865	-0.0138
12	3	12	12	2	11	Δ	5857 3255	0.0086
12	3	12	12	2	11	F	5857 3255	0.0000
10	4	12	12	2 F		L	5057.5255	0.0101
10	4	9	9	5	5	A	5809.8355	0.0132
10	4	9	9	5	5	E	5869.8355	0.0001
6	1	5	5	2	3	A	5881.3360	0.0035
6	1	5	5	2	3	E	5881.3360	0.0069
9	3	8	8	4	4	A	5944.4489	-0.0086
9	3	8	8	4	4	E	5944.4489	-0.0030
12	4	12	12	3	10	А	5946.5173	0.0074
12	4	12	12	3	10	E	5946.5173	0.0100
9	3	8	8	4	5	Δ	5962 4079	-0.0024
0	3	0	0	4	5	F	5962.4079	0.0024
11	3	11	11	4	5	L	5902.4079	0.0008
11	4	11	11	3	9	A	5990.1102	0.0070
11	4	11	11	3	9	E	5996.1162	0.0104
11	2	11	11	1	11	A	6040.9650	-0.0075
11	2	11	11	1	11	E	6040.9650	0.0088
3	2	2	2	1	1	A	6059.6670	-0.0051
3	2	2	2	1	1	E	6059.6670	-0.0042
5	1	4	4	1	4	А	6062.6110	-0.0013
5	1	4	4	1	4	E	6062.6110	0.0000
7	0	6	6	1	5	Ā	6104 0310	0.0039
, 7	0	6	6	1	5	F	6104.0310	0.0000
2	2	2	2	1	1	L	6114 2410	0.0003
3	2	2	2	1	1	A	6114.3419	-0.0061
3	2	2	2	1	1	E	6114.3419	-0.0051
14	5	14	14	4	10	A	6158.2334	0.0074
14	5	14	14	4	10	E	6158.2334	0.0003
13	4	13	13	3	11	A	6163.6748	-0.0065
13	4	13	13	3	11	E	6163.6748	-0.0025
5	0	4	4	0	4	А	6182.6342	-0.0025
5	0	4	4	0	4	F	6182 6342	-0.0011
14	2	14	14	1	13	Δ	6221 4289	-0.0023
1/	2	14	14	1	12	F	6221.4205	0.0025
14 C	2	14	14	2	13	L	6222.4289	0.0104
0	1	5	5	2	4	A	6233.9612	-0.0184
6	1	5	5	2	4	E	6233.9612	-0.0133
13	3	13	13	2	12	A	6328.9923	-0.0012
13	3	13	13	2	12	E	6328.9923	0.0082
9	1	8	8	2	7	A	6337.9098	0.0003
9	1	8	8	2	7	E	6337.9098	-0.0045
5	2	4	4	2	3	А	6351.7760	0.0029
5	2	4	4	2	3	E	6351.7760	0.0051
3	2	2	2	1	2	А	6386.2347	0.0029
3	2	2	2	1	2	F	6386 2347	0.0046
5	_	4	4	-	1	_	6400 9596	-0.0064
5	4	4	4	4	1		6401.0376	-0.0004
5	4	4	4	4	1	E	6401.0376	-0.0025
5	4	4	4	4	0	A	6401.2665	0.0004
5	4	4	4	4	0	E	6401.1823	-0.0050
5	3	4	4	3	2	A	6407.5867	0.0040
5	3	4	4	3	2	E	6407.5867	0.0045
5	3	4	4	3	1	А	6422.1643	-0.0080
5	3	4	4	3	1	E	6422.1643	-0.0035
13	6	12	12	7	5	А	6437.6179	0.0048
3	2	2	2	1	2	A	6440 9065	-0.0012
2	2	2	- 2	1	2	F	6410 9065	0.00012
12	<u>د</u>	∠ 10	ے 12		2	L A	6441 F112	0.0000
14	b	14	14	/	0	A	0441.5113	-0.0017
14	4	14	14	3	12	A -	0441.60/5	-0.0031
14	4	14	14	3	12	E	6441.6075	0.0024
5	1	4	4	0	4	A	6449.7942	-0.0004
5	1	4	4	0	4	E	6449.7942	0.0001
13	5	13	13	4	9	А	6456.0543	-0.0161

12	-	10	12	4	0	-		0 0220
15	5	15	15	4	9	E	0450.0543	-0.0220
12	1	12	12	0	12	A	6463.0911	0.0157
12	1	12	12	0	12	E	6463.0911	0.0100
4	1	3	3	0	3	А	6467.3634	0.0049
4	1	2	2	0	2	F	6467 2624	0.0082
-	2	5	5	2	5	L A	6400,4228	0.0002
9	2	8	8	3	5	A	6490.4228	0.0063
9	2	8	8	3	5	E	6490.4228	0.0053
9	3	8	8	4	5	A	6498.6875	0.0023
9	3	8	8	4	5	E	6498.6875	0.0093
5	2	4	4	2	2	^	6545 2421	0.0054
5	2	4	4	2	2	~	0545.2421	0.0034
5	2	4	4	2	2	E	6545.2421	0.0085
5	1	4	4	1	3	A	6592.2835	0.0007
5	1	4	4	1	3	E	6592.2835	0.0034
12	2	12	12	1	12	Δ	6619 3518	-0.0067
12	2	12	12	1	12	5	6610 2519	0.0107
12	2	12	12	1	12	E	0019.3318	0.0197
8	0	7	7	1	6	A	6645.5420	-0.0115
8	0	7	7	1	6	E	6645.5420	-0.0155
12	5	12	12	4	8	А	6692.3485	0.0122
12	5	12	12	4	8	F	6692 3485	0.0071
12	2			7	c	L A	6052.5485	0.0071
9	2	0	0	3	0	A	6779.6878	-0.0043
9	2	8	8	3	6	E	6779.6878	-0.0033
12	5	11	11	6	5	A	6780.3761	0.0013
12	5	11	11	6	5	E	6780.2730	-0.0037
15	1	15	15	2	12	۸	6780 8011	0.0025
15	4	15	15	2	13	~	0780.8011	0.0025
15	4	15	15	3	13	E	6780.8011	0.0098
13	4	13	13	3	11	A	6841.4284	-0.0127
13	4	13	13	3	11	E	6841.4284	-0.0027
14	3	14	14	2	13	Α	6841 9987	-0.0041
14	2	14	14	2	10	5	6841.0087	0.0076
14	3	14	14	2	13	E	6841.9987	0.0076
11	5	11	11	4	7	A	6864.7828	0.0013
11	5	11	11	4	7	E	6864.7828	-0.0040
10	5	10	10	4	6	А	6982.7721	-0.0098
10	5	10	10	4	6	F	6982 8071	0.0166
10	1	10	10	-	0	L	7012.4001	0.0100
10	1	9	9	2	8	A	7012.4881	0.0020
10	1	9	9	2	8	E	7012.4881	-0.0057
12	5	12	12	4	9	A	7052.2776	0.0010
12	5	12	12	4	9	E	7052.2776	0.0014
٩	5	٩	٩	4	5	Δ	7058 0993	-0.0251
0	5	0	5	4	5	- -	7058.0555	0.0251
9	5	9	9	4	5	E	7058.0993	-0.0059
9	5	9	9	4	5	A	7059.8715	-0.0163
9	5	9	9	4	5	E	7059.9120	0.0032
11	5	11	11	4	8	А	7060.7624	0.0004
11	5	11	11	4	8	F	7060 7624	0.0019
12	5	12	12	4	10	L A	7000.7024	0.0015
15	5	15	15	4	10	A .	7003.7302	0.0007
13	5	13	13	4	10	E	7063.7302	0.0008
10	5	10	10	4	7	A	7080.2649	0.0106
10	5	10	10	4	7	Е	7080.2649	0.0162
6	0	5	5	1	5	Δ	7081 3854	-0.0027
c	0	5	5	1	5	- -	7081.3854	0.0027
0	0	5	3	1	5	E .	7081.3854	-0.0002
11	4	10	10	5	5	A	/082.4/93	-0.0290
11	4	10	10	5	5	E	7082.4793	-0.0155
7	1	6	6	2	4	А	7096.7089	-0.0086
7	1	6	6	2	4	F	7096 7089	-0.0059
,	-	0	0	2	-	L A	7030.7003	0.0000
9	5	9	9	4	0	A	/103.6/51	-0.0089
9	5	9	9	4	6	E	7103.6751	0.0097
14	5	14	14	4	11	A	7105.1948	0.0009
14	5	14	14	4	11	Е	7105.1948	0.0015
13	1	13	13	0	13	Δ	7116 2136	0.0087
10	1	13	10	0	13	-	7110.2150	0.0007
13	T	13	13	0	13	E	/116.2136	-0.0163
8	5	8	8	4	4	E	7108.1509	-0.0063
8	5	8	8	4	4	A	7108.2202	-0.0004
8	5	8	8	4	4	А	7108,7229	-0.0068
8	5	8	8	4	1	F	7108 7908	-0.0019
0	5	0	0	-	-		7100.7500	0.0015
8	5	8	8	4	5	A	/126.1615	-0.0119
8	5	8	8	4	5	E	7126.1123	-0.0001
8	5	8	8	4	5	А	7126.7019	0.0194
8	5	8	8	4	5	E	7126.7491	0.0012
9	0	8	8	1	7	Δ	7126 8938	0.0161
0	0	0	0	1	7	-	7120.0330	0.0101
9	U	ŏ	ŏ	1	/	E	/120.8938	0.0117
7	5	7	7	4	3	A	7138.8732	-0.0009
7	5	7	7	4	3	E	7138.7288	-0.0020
7	5	7	7	4	3	А	7138.9927	0.0003
. 7	5	7	7		2	F	7120 1205	
, ,	5	7	7	4	ر م	L ^	7133.1233	0.0003
/	5	/	/	4	4	A	/144.9624	0.0042
7	5	7	7	4	4	E	7144.8244	0.0020
7	5	7	7	4	4	А	7145.0815	0.0049
7	5	7	7	4	4	E	7145.2249	0.0033

10	3	9	9	4	5	А	7148.0324	0.0008
10	3	9	9	4	5	E	7148.0324	0.0053
6	5	6	6	4	2	А	7157.3575	0.0341
6	5	6	6	4	2	E	7157.1326	0.0034
6	5	6	6	4	2	А	7157.3575	0.0143
6	5	6	6	4	2	E	7157.5195	0.0079
6	5	6	6	4	3	А	7158.9927	-0.0081
6	5	6	6	4	3	E	7158.8261	-0.0080
6	5	6	6	4	3	А	7158.9927	-0.0279
6	5	6	6	4	3	E	7159.2081	-0.0084
5	5	5	5	4	1	А	7168.1140	-0.0037
5	5	5	5	4	1	E	7167.8571	-0.0123
5	5	5	5	4	1	А	7168.1140	-0.0055
5	5	5	5	4	1	E	7168.2463	-0.0054
5	5	5	5	4	2	A	7168.4493	-0.0062
5	5	5	5	4	2	E	7168.3238	-0.0010
5	5	5	5	4	2	A	7168.4493	-0.0080
5	5	5	5	4	2	E	7168.6997	-0.0074
4	2	3	3	1	2	A	7170.3317	-0.0016
4	2	3	3	1	2	E	7170.3317	-0.0008
9	2	9	9	1	9	А	7182.8827	-0.0137
9	2	9	9	1	9	E	7182.8827	0.0028
15	5	15	15	4	12	A	7186.8927	-0.0002
15	5	15	15	4	12	E	7186.8927	0.0013
10	3	9	9	4	6	Α	7193.5801	-0.0112
10	3	9	9	4	6	E	7193.5801	-0.0072
10	2	9	9	3	6	Α	7200.5676	-0.0015
10	2	9	9	3	6	E	7200.5676	-0.0051
13	2	13	13	1	13	Α	7211.3235	-0.0136
13	2	13	13	1	13	E	7211.2813	-0.0085
8	2	7	7	3	4	Α	7216.1222	-0.0008
8	2	7	7	3	4	E	7216.1222	0.0065
6	1	5	5	1	5	Α	7254.1603	0.0070
6	1	5	5	1	5	E	7254.1603	0.0085
11	4	10	10	5	6	A	7297.3482	0.0140
11	4	10	10	5	6	E	7297.3482	0.0158
16	5	16	16	4	13	А	7318.1448	0.0207
16	5	16	16	4	13	E	7318.1021	-0.0192
4	2	3	3	1	2	Α	7329.5141	-0.0028
4	2	3	3	1	2	E	7329.5141	-0.0012
6	0	5	5	0	5	Α	7348.5508	0.0049
6	0	5	5	0	5	E	7348.5508	0.0064

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J	K'a	K′c	J″	K"a	К"с	Symm.	Obs./MHz	Diff./MHz
4	1	3	3	2	1	А	2071.8751	0.0007
4	1	3	3	2	1	E	2071.8751	0.0012
7	1	6	7	0	7	А	2188.8734	0.0001
7	1	6	7	0	7	F	2188 8734	0.0025
, 1	1	1	,	0	,	~	2100.07.54	0.0025
1	1	1	0	0	0	A	2189.3043	-0.0037
1	1	1	0	0	0	E	2189.3643	0.0011
7	2	6	7	1	6	A	2191.6419	-0.0050
7	2	6	7	1	6	E	2191.6419	0.0074
1	1	0	0	0	0	Α	2254.2047	-0.0037
1	1	0	0	0	0	E	2254.2047	-0.0005
6	2	4	5	3	2	Δ	2313 09/6	-0.0007
c	2	4	5	2	2	- -	2313.0540	0.0007
0	2	4	5	5	2	Ē	2312.9581	-0.0023
6	2	5	6	1	5	A	2395.9423	-0.0080
6	2	5	6	1	5	E	2395.9423	0.0049
5	1	5	4	2	2	Α	2426.5207	0.0101
5	1	5	4	2	2	E	2426.5207	0.0032
3	0	3	2	1	1	Α	2486.6213	0.0004
3	0	3	2	1	1	F	2486 6213	-0.0030
0	2	5	2	1		L	2480.0213	0.0050
0	2	0	0	1	/	A	2343.3337	-0.0128
8	2	6	8	1	/	E	2545.3357	-0.0035
7	2	5	7	1	6	A	2552.9781	-0.0065
7	2	5	7	1	6	E	2552.9781	0.0035
5	2	4	5	1	4	А	2576.9349	-0.0054
5	2	4	5	1	4	E	2576.9349	0.0084
8	1	7	8	0	8	Δ	2590 6758	-0.0014
0	1	7	0	0	0	- -	2550.0758	0.00014
0	1	/	0	0	0	Ē	2590.0758	0.0005
9	2	/	9	1	8	A	2591.6249	-0.0025
9	2	7	9	1	8	E	2591.6249	0.0059
6	2	4	6	1	5	Α	2603.2423	-0.0163
6	2	4	6	1	5	E	2603.2423	-0.0060
8	3	5	7	4	3	Α	2611.6245	-0.0005
8	3	5	7	4	3	F	2610 9583	-0.0018
2	0	2	,	1	2	~	2610.5505	0.0024
5	0	5	2	1	2	A	2081.1440	0.0024
3	0	3	2	1	2	E	2681.1446	-0.0016
5	2	3	5	1	4	A	2682.8870	-0.0085
5	2	3	5	1	4	E	2682.8870	0.0013
10	2	8	10	1	9	А	2701.0841	-0.0026
10	2	8	10	1	9	E	2701.0841	0.0046
4	2	3	4	1	3	Δ	2731 3826	0.0127
4	2	2	4	1	2	F	2721 2//1	-0.0097
4	2	3	4	1	3	Ē	2/31.3441	-0.0097
4	2	2	4	1	3	A	2777.3848	-0.0070
4	2	2	4	1	3	E	2777.3848	0.0007
3	2	2	3	1	2	Α	2856.9783	-0.0016
3	2	2	3	1	2	E	2856.9481	-0.0075
3	2	1	3	1	2	А	2872.4367	0.0071
3	2	1	3	1	2	F	2872 4367	0.0068
11	-	-	11	-	10	~	200211000	0.0030
11	2	9	11	1	10	A	2881.2324	-0.0030
11	2	9	11	1	10	E	2881.2324	0.0027
9	1	8	9	0	9	A	3055.7852	0.0026
9	1	8	9	0	9	E	3055.7852	0.0041
12	2	10	12	1	11	A	3137.7103	-0.0011
12	2	10	12	1	11	E	3137.7103	0.0031
3	2	2	3	1	3	Δ	3245 9401	0.0110
2	2	2	2	1	2	F	22/15/19/17	-0.0075
5	2	2	5	1	5	E A	3243.8977	-0.0073
3	2	1	3	1	3	A	3261.3803	0.0016
3	2	1	3	1	3	E	3261.3803	0.0008
7	2	6	6	3	3	A	3267.3308	-0.0182
7	2	6	6	3	3	E	3267.3308	0.0181
7	2	6	6	3	4	А	3275.0742	0.0018
7	2	6	6	3	4	F	3275 1454	-0.0002
ว	- 1	2	1	0	1	Δ	3329 8025	-0 0042
2	1	2	1	0	1		3329.8025	-0.0042
2	1	2	1	U	1	E	3329.8025	0.0001
6	1	6	5	2	3	A	3361.8998	0.0077
6	1	6	5	2	3	E	3361.8998	-0.0012
4	2	3	4	1	4	А	3379.1037	-0.0198
4	2	3	4	1	4	Е	3379.1037	-0.0040
5	1	4	4	2	2	Δ	3396 5301	0.0058
5	1	4	4	2	2	с. Г	3306 5201	_0 0017
5	1	4	4	2	2	E .	3330.3301	-0.0017
4	2	2	4	1	4	A	3425.1368	-0.0086
4	2	2	4	1	4	E	3425.1368	-0.0013
5	1	4	4	2	3	Α	3442.5354	-0.0109
5	1	4	4	2	3	E	3442.5678	0.0056
13	2	11	13	1	12	А	3473.5233	-0.0022

Table S11: Line list for the fit obtained using the XIAM program for *trans*-out-perp conformer, measured rotational transitions are shown as Obs. and the residuals are shown as Diff.

	_					_		
13	2	11	13	1	12	E	3473.5233	0.0003
2	1	1	1	0	1	А	3524.3183	-0.0096
2	1	1	1	0	1	F	3524 3183	-0.0059
-	2	1	-	1	-	-	3524.5105	0.0000
5	2	4	5	1	5	А	3546.9571	0.0030
5	2	4	5	1	5	E	3546.9571	0.0163
4	0	4	3	1	2	А	3566.0319	-0.0108
4	0	4	2	1	2	E	2566 0210	0.01.41
4	0	4	5	1	2	E	3300.0319	-0.0141
10	1	9	10	0	10	A	3575.5153	-0.0017
10	1	9	10	0	10	E	3575.5153	-0.0005
7	2	E	6	2	2	۸	2620 6744	0.0122
<i>'</i>	2	5	0	5	5	A	5028.0744	-0.0125
7	2	5	6	3	3	E	3628.6744	0.0215
7	2	5	6	3	4	Α	3636.4062	-0.0038
7	2	5	6	2	4	F	2626 4615	-0.0244
/	2	5	0	5	4	E	5050.4015	-0.0244
5	2	3	5	1	5	A	3652.9008	-0.0084
5	2	3	5	1	5	E	3652.9008	0.0009
6	2	E	6	1	6	۸	2740 9562	0.0049
0	2	5	0	1	0	A	3749.6303	-0.0046
6	2	5	6	1	6	E	3749.8563	0.0075
9	3	7	8	4	5	Α	3786.5611	-0.0051
0	2	7	0	1	5	F	2787 0652	0.0040
9	5	/	0	4	5	E	3787.0033	0.0040
14	2	12	14	1	13	A	3887.9492	0.0022
14	2	12	14	1	13	E	3887.9492	0.0031
4	0	4	2	1	2	۸	2054 0041	0.0022
4	0	4	5	T	5	A	5954.9941	0.0025
4	0	4	3	1	3	E	3954.9941	-0.0015
6	2	4	6	1	6	А	3957.1642	-0.0052
6	2	1	6	1	6	F	2057 1642	0.0044
0	2	4	0	1	0	L .	3937.1042	0.0044
7	2	6	7	1	7	A	3987.9834	0.0075
7	2	6	7	1	7	E	3987,9834	0.0193
11	1	10	11	_	11	_	4127 6407	0.0014
11	T	10	11	0	11	A	4137.0497	0.0014
11	1	10	11	0	11	E	4137.6497	0.0025
7	1	7	6	2	4	А	4217.5961	0.0056
-	-	-	c c	2		5	121715561	0.0005
/	1	/	6	2	4	E	4217.5961	-0.0035
8	2	7	8	1	8	A	4260.9571	-0.0227
8	2	7	8	1	8	F	4260 9571	-0.0112
-	2	,	-	1	-	-	4200.5571	0.0112
/	2	5	/	1	/	A	4349.3035	-0.0101
7	2	5	7	1	7	E	4349.3035	-0.0008
15	2	13	15	1	14	Δ	4375 6485	-0.0022
15	2	15	15	-	14	2	4373:0483	0.0022
15	2	13	15	1	14	E	4375.6485	-0.0028
8	2	7	7	3	4	Α	4403.3025	-0.0081
8	2	7	7	3	4	F	4403 3025	-0.00/13
0	2	,	,	5	-	-	4405.5025	0.0045
8	2	/	/	3	5	A	4422.5033	0.0193
8	2	7	7	3	5	E	4422.5033	-0.0212
7	1	7	6	2	5	Δ	1121 9018	0.0059
<i>'</i>	1	<i>'</i>	0	2	5	~	4424.9048	0.0039
7	1	7	6	2	5	E	4424.9048	-0.0058
3	1	3	2	0	2	Α	4439.0266	-0.0022
2	1	2	2	0	2	F	4439 0266	0.0020
5	1	5	2	0	2	L .	4433.0200	0.0020
9	3	7	9	2	7	A	4474.4467	0.0024
9	3	7	9	2	7	E	4474.4129	-0.0043
٥	2	6	٥	2	7	۸	4556 6207	0.0067
5	5	0	9	2	,	~	4550.0237	0.0007
9	3	6	9	2	/	E	4556.6297	0.0229
9	2	8	9	1	9	Α	4568.0003	0.0023
٩	2	8	٩	1	٩	F	4568 0003	0.0136
5	2	-		-	5	-	4508.0005	0.0150
5	0	5	4	1	3	A	4588.1479	-0.0114
5	0	5	4	1	3	E	4588.1479	-0.0145
8	3	6	8	2	6	Δ	4669 2083	0 0007
~	2	с С	0	-	с С	-	100512000	0.0007
ð	3	b	8	2	6	E	4009.1/39	-0.0021
8	3	5	8	2	6	A	4710.9369	-0.0043
8	3	5	8	2	6	F	4710 9369	0.0068
6	5	5	5	2	0	-	4710.5505	0.0000
6	1	5	5	2	3	A	4715.8101	0.0072
6	1	5	5	2	3	E	4715.8101	-0.0023
12	1	11	12	0	12	Δ	1728 2017	-0.00/18
12	1	11	12	0	12	2	4720.2047	0.0040
12	1	11	12	0	12	E	4728.2047	-0.0036
7	3	5	7	2	5	Α	4820.7068	-0.0050
7	3	5	7	2	5	F	4820 6711	0.0026
,	5	5	,	2	5		4020.0711	0.0020
6	1	5	5	2	4	A	4821.7642	0.0061
6	1	5	5	2	4	E	4821.7642	-0.0074
з	1	2	2	Ο	2	Δ	4827 9753	-0 0027
5	-	~	~	0	2	~	4027.3733	0.0027
3	1	2	2	0	2	E	4827.9753	0.0012
8	2	6	8	1	8	А	4837.8065	-0.0047
8	С	6	8	1	<u>e</u>	F	1837 9065	0.0040
о _	2	U	0	T	0	E	4037.0000	0.0040
7	3	4	7	2	5	A	4839.8793	-0.0059
7	3	4	7	2	5	E	4839.8793	-0.0069
10	-	0	10	- 1	10	^	1007 5272	_0.0109
10	2	9	10	1	10	A	4907.3373	-0.0108
10	2	9	10	1	10	E	4907.5373	0.0004
6	3	4	6	2	4	А	4930.4939	-0.0001
6	2	Λ	6	э	Λ	F	1930 1212	0.0062
0	5	4	0	2	4	E (4330.4242	0.0002
6	3	3	6	2	4	A	4938.2396	0.0221
6	3	3	6	2	4	E	4938.2396	-0.0114

•	2	6	-	2			1000 1 100	0.0014
8	2	6	/	3	4	A	4980.1406	-0.0014
8	2	6	7	3	4	E	4980.1406	-0.0004
8	1	8	7	2	5	А	4982.2260	0.0100
8	1	8	7	2	5	F	1982 2576	0 0330
0	2	6	, ,	2	5	-	4000 2520	0.0000
8	2	6	/	3	5	E	4999.3526	-0.0062
10	3	8	9	4	6	A	5000.6541	0.0060
10	3	8	9	4	6	E	5000.9189	0.0073
5	3	3	5	2	3	А	5003.3852	0.0047
5	2	2	F	2	2	E	E002 2101	0.0074
5	5	5	5	2	5	E .	5005.2101	0.0074
5	3	2	5	2	3	A	5005.9664	0.0002
5	3	2	5	2	3	E	5006.1019	0.0017
4	3	2	4	2	2	А	5046.7375	0.0088
1	3	2	1	2	2	F	50/6 2979	-0.0006
-	2	2	4	2	2	L	5040.2373	0.0000
4	3	1	4	2	2	A	5047.3750	-0.0017
4	3	1	4	2	2	E	5047.7614	0.0024
3	3	1	3	2	1	Α	5068.9635	-0.0056
3	3	1	3	2	1	E	5068.3273	0.0003
2	2	0	2	2	1	^	5069 0620	0.0002
5	3	0	5	2	1	~	5005.0020	0.0002
3	3	0	3	2	1	E	5069.6434	0.0036
3	3	1	3	2	2	A	5084.4143	-0.0045
3	3	1	3	2	2	E	5083.8031	0.0018
3	з	0	3	2	2	Δ	5084 5110	-0 0004
2	2	0	2	-	-		500 1161	0.0020
5	5	0	3	2	2	E	5085.1101	0.0020
4	3	2	4	2	3	A	5092.7476	-0.0031
4	3	2	4	2	3	E	5092.3268	-0.0021
4	3	1	4	2	3	А	5093.3988	0.0001
1	3	1	1	2	3	F	5093 7923	0 0030
-	3	1	4	2	5	L	5095.7925	0.0030
5	3	3	5	2	4	A	5109.3356	0.0000
5	3	3	5	2	4	E	5109.1612	-0.0007
5	3	2	5	2	4	Α	5111.9226	0.0012
5	3	2	5	2	4	F	5112 0612	0.0018
c	2	4	c	2	-	~	5112.0012	0.0010
o	3	4	0	Z	5	А	5137.8002	-0.0022
6	3	4	6	2	5	E	5137.7271	-0.0019
6	3	3	6	2	5	А	5145.5317	0.0059
6	3	3	6	2	5	E	5145.5640	0.0020
7	2	5	7	2	6	^	5182 0228	-0.0257
<i>'</i>	3	5	,	2	0	~	5182.0238	-0.0237
/	3	5	/	2	6	E	5182.0238	0.0152
7	3	4	7	2	6	A	5201.2230	0.0000
7	3	4	7	2	6	E	5201.2230	-0.0034
5	0	5	4	1	4	А	5235.9150	0.0022
5	0	5	1	1	1	F	5225 0150	-0.0012
5	0	5	4	1	4	L	5255.5150	-0.0013
8	3	6	8	2	/	A	5246.0400	0.0010
8	3	6	8	2	7	E	5246.0082	-0.0019
11	2	10	11	1	11	Α	5277.5525	-0.0011
11	2	10	11	1	11	F	5277 5525	0.0102
0	2	10		2		~	5277.5525	0.0102
0	3	5	0	2	/	A	5287.7711	-0.0015
8	3	5	8	2	7	E	5287.7711	0.0068
8	1	8	7	2	6	A	5343.5604	0.0068
8	1	8	7	2	6	E	5343.5604	-0.0044
9	3	6	9	2	8	Δ	5415 7683	-0.0029
0	2	c	0	-	0		5415 7693	0.0000
9	3	0	9	2	0	E	5415.7683	0.0099
9	2	/	9	1	9	A	5427.1469	0.0007
9	2	7	9	1	9	E	5427.1469	0.0085
2	2	1	1	1	0	А	5427.6615	0.0027
2	2	1	1	1	0	F	5427 5887	0 0028
2	2	- -	1		0	~	E420 7645	0.0020
2	2	U	1	1	U	A _	5430.7645	0.0064
2	2	0	1	1	0	E	5430.8079	0.0022
10	3	8	10	2	9	A	5448.2114	0.0078
10	3	8	10	2	9	E	5448.1626	-0.0201
2	2	1	1	1	1	Δ	5/192 5072	0.0079
2	2	1	1	1	1	-	5402.3072	0.0075
2	2	1	1	1	1	E	5492.4313	0.0035
9	2	8	8	3	5	A	5504.5055	-0.0039
9	2	8	8	3	5	E	5504.5055	-0.0116
4	1	4	3	0	3	А	5521.0384	-0.0030
4	1	4	2	0	2	F	5521 0384	0 0012
ć	-	-	5	4	ر ۸	L ^	5521.0504	0.0013
o	U	ь	5	T	4	A	5544.4442	0.0094
6	0	6	5	1	4	E	5544.4442	0.0068
11	3	9	11	2	10	А	5592.8853	0.0096
11	3	9	11	2	10	E	5592.8421	-0.0144
10	2	7	10	2	 0	^	5597 5171	0.0019
10	5	,	10	2	5	~	5557.5171	0.0010
10	3	/	10	2	9	E	5597.5171	0.0159
14	1	13	14	0	14	A	5942.0081	-0.0001
14	1	13	14	0	14	E	5942.0081	0.0014
13	3	11	13	2	12	А	5981,1866	-0 0152
13	2	11	12	2	12	F	5981 1966	0 0010
10	5	11	12	2	12	Ľ	5361.1000	0.0019
15	4	12	15	3	12	A	6010.2819	-0.0145
15	4	12	15	3	12	E	6010.2819	0.0239

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/	1	6	6	2	4	A	6013.9210	0.0015
7	1	6	6	2	4	E	6013.9210	-0.0082
10	2	8	10	1	10	А	6117.7449	0.0062
10	2	8	10	1	10	F	6117 7449	0.0133
10	-	2	20	-	20	-	6160 7065	0.0135
4	1	3	3	0	3	A	0108.7905	0.0016
4	1	3	3	0	3	E	6168.7965	0.0055
7	1	6	6	2	5	A	6221.2409	0.0131
7	1	6	6	2	5	E	6221.2409	0.0007
9	2	7	8	з	5	Δ	6363 6659	0 0084
0	2	, 7	0	2	5		6363.6655	0.0004
9	2	/	8	3	5	E	6363.6659	-0.0028
/	0	/	6	1	5	A	6428.3088	0.0041
7	0	7	6	1	5	E	6428.3088	0.0021
6	0	6	5	1	5	А	6514.4494	0.0008
6	0	6	5	1	5	F	6514 4494	-0.0023
12	4	10	12	2	10	~	6524.0225	0.0023
15	4	10	15	5	10	A	0324.9223	-0.0104
3	2	2	2	1	1	A	6568.1113	0.0195
3	2	2	2	1	1	E	6568.0708	0.0036
5	1	5	4	0	4	А	6582.1601	-0.0035
5	1	5	1	0	1	F	6582 1601	0.0008
2	2	1	7	1	1	L A	6582.1001	0.0000
3	2	1	2	1	1	A	0583.5437	0.0022
3	2	1	2	1	1	E	6583.5437	0.0021
12	4	8	12	3	9	A	6734.9709	-0.0028
12	4	8	12	3	9	E	6734.9709	0.0020
3	2	2	2	1	2	А	6762.6243	0.0112
2	2	2	2	-	2	F	6762 5787	-0.0104
5	2	2	2	1	2	L	6772.0787	-0.0104
3	2	1	2	1	2	A	6778.0634	0.0007
3	2	1	2	1	2	E	6778.0634	0.0000
11	4	8	11	3	8	А	6842.8511	-0.0020
11	4	8	11	3	8	E	6842.7649	-0.0055
10	1	7	10	3	7	Δ	6940 5671	0.0096
10	4	, ,	10	2	, ,	-	6040.4262	0.0050
10	4	/	10	3	/	E	6940.4262	0.0094
10	4	6	10	3	7	A	6947.3117	-0.0112
10	4	6	10	3	7	E	6947.3972	-0.0036
9	4	6	9	3	6	А	7007.5635	-0.0075
9	4	6	9	3	6	F	7007 2902	-0.0086
0	1	5	0	2	6	_	7010 4845	-0.0062
5	4	5	3	3	0	2	7010.4845	-0.0002
9	4	5	9	3	0	E	7010.6939	-0.0024
8	4	5	8	3	5	A	/051.5358	0.0003
8	4	5	8	3	5	E	7051.0223	-0.0023
8	4	4	8	3	5	A	7052.6640	-0.0001
8	4	4	8	3	5	Е	7053.0990	0.0001
10	1	10	9	2	8	Δ	7068 2427	0 0039
10	1	10	0	2	0	5	7068.2427	0.0000
10	1	10	9	2	0	E	/068.242/	-0.0066
/	4	4	/	3	4	A	/0/9.0///	-0.0029
7	4	4	7	3	4	E	7078.3318	0.0037
7	4	3	7	3	4	А	7079.4728	0.0146
7	4	3	7	3	4	E	7080.1098	-0.0012
0	1	5	0	2	7	_	7092 6711	0.0015
9	4	5	5	2	7	~	7092.0711	0.0013
9	4	5	9	3	/	E	7092.8936	0.0077
8	4	5	8	3	6	A	7093.2713	0.0022
8	4	5	8	3	6	E	7092.7883	0.0096
8	4	4	8	3	6	А	7094.3979	0.0002
8	1	4	8	3	6	F	709/ 8555	0.0025
c	4	-	c	2	2	L A	7054.0555	0.0025
0	4	5	0	5	5	A	7095.4696	0.0023
6	4	3	6	3	3	E	/094.5852	0.0021
6	4	2	6	3	3	A	7095.5898	-0.0007
6	4	2	6	3	3	E	7096.3320	0.0021
11	4	8	11	3	9	А	7096 4505	-0 0091
10		6	10	2	0	^	7006 6210	0.0129
10	4	0	10	3	8	2	7090.0210	-0.0138
10	4	6	10	3	8	E	/096./04/	-0.0146
7	4	4	7	3	5	A	7098.2438	-0.0102
7	4	4	7	3	5	E	7097.5377	-0.0081
7	4	3	7	3	5	А	7098.6335	0.0019
7	4	3	7	3	5	F	7099 3280	-0.0006
	1	2	, F	2	1	Δ	7102 21/7	0.0000
6	4	с С	6	с С	4	-	7103.2147	0.0039
D C	4	3	D	3	4	Ē	/102.4105	-0.0055
6	4	2	6	3	4	A	/103.3138	-0.0002
6	4	2	6	3	4	E	7104.1671	0.0042
5	4	1	5	3	2	А	7104.6830	-0.0292
5	4	1	5	3	2	E	7105.3922	0.0015
5	4	2	5	3	2	Δ	7104 6830	-0.0085
5		2	5	2	2		7102 6761	0.0005
5	4	4	5	с С	2	L ^	7107 2001	0.0303
5	4	Ţ	5	3	3	A	/10/.3001	0.0022
5	4	1	5	3	3	Ē	/108.2897	0.0014
5	4	2	5	3	3	A	7107.3001	0.0229
5	4	2	5	3	3	Е	7106.5407	-0.0027
4	4	0	4	3	1	А	7109.4685	-0.0049

4	4	0	4	3	1	E	7109.9086	-0.0024
4	4	1	4	3	1	А	7109.4685	-0.0026
4	4	1	4	3	1	E	7108.1510	-0.0148
4	4	1	4	3	2	А	7110.1175	-0.0017
4	4	1	4	3	2	E	7109.6216	-0.0046
4	4	0	4	3	2	А	7110.1175	-0.0040
12	4	8	12	3	10	А	7141.3109	0.0165
12	4	8	12	3	10	E	7141.3109	0.0162
8	0	8	7	1	6	А	7236.9878	0.0017
8	0	8	7	1	6	E	7236.9878	0.0004
8	1	7	7	2	5	А	7274.6974	0.0187
8	1	7	7	2	5	E	7274.6974	0.0093
5	1	4	4	0	4	A	7552.1723	-0.0051
5	1	4	4	0	4	E	7552.1723	-0.0013
6	1	6	5	0	5	A	7630.5315	-0.0130
6	1	6	5	0	5	E	7630.5315	-0.0087
8	1	7	7	2	6	A	7636.0275	0.0111
8	1	7	7	2	6	E	7636.0275	-0.0007
4	2	3	3	1	2	A	7675.6660	-0.0079
4	2	3	3	1	2	E	7675.6660	0.0085
4	2	2	3	1	2	A	7721.6859	-0.0099
4	2	2	3	1	2	E	7721.6859	-0.0020
10	2	8	9	3	6	A	7770.2043	-0.0019
10	2	8	9	3	6	E	7770.2043	-0.0181
7	0	7	6	1	6	A	7782.2122	-0.0033
7	0	7	6	1	6	E	7782.2122	-0.0059
9	0	9	8	1	7	A	7972.5331	-0.0040
9	0	9	8	1	7	E	7972.5331	-0.0046