

# **Conformational Behaviour of Norephedrine, Ephedrine, and Pseudoephedrine**

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Table S1. Experimental rotational parameters for the observed conformers of norephedrine.

EXPERIMENTAL	AG	GG	GA
A <sup>a</sup> /MHz	2330.15332(22) <sup>d</sup>	1856.19039(80)	2210.38150(76)
B /MHz	676.963452(41)	791.01512(14)	696.642553(62)
C /MHz	637.669563(43)	709.15405(14)	627.302876(54)
$\Delta_J$ /kHz	0.03807(48)	0.0617(16)	0.03914(47)
$\Delta_{JK}$ /kHz	0.1041(38)	-	-
$\chi_{aa}$ /MHz	2.3837(28)	1.681(19)	1.659(15)
$\chi_{bb}$ /MHz	-3.8821(25)	-3.627(12)	1.7497(99)
$\chi_{cc}$ /MHz	1.4984(25)	1.946(12)	-3.4087(99)
N <sup>b</sup>	88	33	41
$\sigma^c$ / kHz	1.1	2.1	1.1

<sup>a</sup> A, B and C are the rotational constants,  $\Delta_J$ ,  $\Delta_{JK}$ , and  $\delta_J$  are the quartic centrifugal distortion constants, and  $\chi_{aa}$ ,  $\chi_{bb}$ , and  $\chi_{cc}$  are elements of the <sup>14</sup>N nuclear quadrupole coupling tensor. <sup>b</sup> Number of fitted hyperfine components. <sup>c</sup> Rms deviation of the fit. <sup>d</sup> Standard error in parentheses in units of the last digit.

Table S2. Experimental rotational parameters for the observed conformers of ephedrine.

EXPERIMENTAL	AGa	AGb	GGa
A <sup>a</sup> /MHz	1998.63816(36) <sup>d</sup>	2115.87676(60)	1568.24542(47)
B /MHz	529.549516(44)	503.794270(41)	592.448481(69)
C /MHz	500.160018(43)	475.173400(51)	572.416000(73)
$\Delta_J$ /kHz	0.01926(39)	0.01822(31)	0.05372(51)
$\Delta_{JK}$ /kHz	0.0674(64)	-	-0.1494(86)
$\delta_J$ / kHz	-	-	-0.00293(38)
$\chi_{aa}$ /MHz	2.5350(14)	2.559(17)	2.4480(89)
$\chi_{bb}$ /MHz	-2.7448(19)	-4.621(11)	-3.2053(63)
$\chi_{cc}$ /MHz	0.2098(19)	2.062(11)	0.7573(63)
N <sup>b</sup>	87	83	98
$\sigma^c$ / kHz	1.3	1.3	1.9

<sup>a</sup> A, B and C are the rotational constants,  $\Delta_J$ ,  $\Delta_{JK}$ , and  $\delta_J$  are the quartic centrifugal distortion constants, and  $\chi_{aa}$ ,  $\chi_{bb}$ , and  $\chi_{cc}$  are elements of the <sup>14</sup>N nuclear quadrupole coupling tensor. <sup>b</sup> Number of fitted hyperfine components. <sup>c</sup> Rms deviation of the fit. <sup>d</sup> Standard error in parentheses in units of the last digit.

Table S3. Experimental rotational parameters for the observed conformers of pseudoephedrine.

EXPERIMENTAL	AGa	AGb	GGa	GGb
A <sup>a</sup> /MHz	2013.35560(27) <sup>d</sup>	2065.86584(17)	1645.9858(13)	1638.6903(23)
B /MHz	509.245110(80)	528.726489(56)	563.58807(46)	602.37256(22)
C /MHz	476.304851(82)	485.202523(53)	541.52877(47)	587.11272(25)
$\Delta_J$ /kHz	0.02274(64)	0.01929(41)	0.0404(44)	0.0455(20)
$\chi_{aa}$ /MHz	2.7231(78)	2.6577(48)	1.355(54)	1.987(70)
$\chi_{bb}$ /MHz	-4.5244(61)	-4.1185(40)	-0.329(34)	-0.185(46)
$\chi_{cc}$ /MHz	1.8013(61)	1.4608(40)	-1.026(34)	-1.803(46)
N <sup>b</sup>	66	55	19	22
$\sigma^c$ / kHz	2.1	1.2	4.1	2.5

<sup>a</sup> A, B and C are the rotational constants,  $\Delta_J$ ,  $\Delta_{JK}$ , and  $\delta_J$  are the quartic centrifugal distortion constants, and  $\chi_{aa}$ ,  $\chi_{bb}$ , and  $\chi_{cc}$  are elements of the <sup>14</sup>N nuclear quadrupole coupling tensor. <sup>b</sup> Number of fitted hyperfine components. <sup>c</sup> Rms deviation of the fit. <sup>d</sup> Standard error in parentheses in units of the last digit.

Table S4. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer AG of norephedrine.

$J'$	$K'_{-l}$	$K'_{+l}$	$J''$	$K''_{-l}$	$K''_{+l}$	$F'$	$F''$	<i>wbs</i>	<i>wbs-wcal</i>
3	1	3	2	0	2	4	3	5499.353	-0.002
						3	2	5498.302	0.000
						2	1	5499.878	0.001
3	1	2	2	0	2	4	3	5734.664	0.002
						3	2	5735.402	0.000
						2	1	5734.554	-0.002
4	0	4	3	0	3	5	4	5251.607	-0.001
						4	3	5251.581	0.000
						3	2	5251.684	0.000
4	1	4	3	1	3	5	4	5178.560	0.000
						4	3	5178.624	0.000
						3	2	5178.516	0.001
4	1	4	3	0	3	5	4	6736.805	-0.002
						4	3	6735.822	0.000
						3	2	6737.131	0.002
4	1	3	3	0	3	5	4	7129.207	0.005
						4	3	7130.055	0.002
						3	2	7129.054	0.000
5	0	5	4	0	4	6	5	6559.371	0.000
						5	4	6559.326	-0.001
						4	3	6559.416	0.001
5	1	5	4	1	4	6	5	6471.957	0.000
						5	4	6471.981	0.000
						4	3	6471.938	-0.001
5	2	4	4	2	3	6	5	6571.553	-0.001
						5	4	6571.713	0.000
						4	3	6571.538	-0.001
5	2	3	4	2	2	6	5	6585.317	0.000
						5	4	6585.534	0.000
						4	3	6585.296	0.001
5	3	3	4	3	2	6	5	6575.336	0.001
						5	4	6575.712	0.001
						4	3	6575.245	0.000
5	3	2	4	3	1	6	5	6575.495	0.000
						5	4	6575.874	0.002
						4	3	6575.402	-0.002
5	1	5	4	0	4	6	5	7957.153	-0.003
						5	4	7956.222	0.000
						4	3	7957.385	0.001
5	1	4	4	0	4	6	5	8545.836	0.003
						5	4	8546.759	-0.002
						4	3	8545.682	-0.001
6	0	6	5	0	5	7	6	7863.785	0.000
						6	5	7863.729	0.001
						5	4	7863.821	0.000

Table S4 (cont.). Observed frequencies and residuals (in MHz) for the rotational transitions of conformer AG of norephedrine.

$J'$	$K'_{-1}$	$K'_{+1}$	$J''$	$K''_{-1}$	$K''_{+1}$	$F'$	$F''$	$\omega_{bs}$	$\omega_{bs}-\omega_{cal}$
6	1	5	5	1	4	7	6	7999.871	-0.001
						6	5	7999.897	0.000
						5	4	7999.925	-0.001
						6	6	8001.538	-0.001
						5	5	7997.949	0.000
6	2	5	5	2	4	7	6	7884.617	-0.001
						5	4	7884.617	-0.001
						6	5	7884.707	0.000
6	2	4	5	2	3	7	6	7908.586	0.000
						6	5	7908.742	0.000
						5	4	7908.580	-0.001
						6	6	7909.377	-0.001
						5	5	7907.815	-0.001
6	3	4	5	3	3	7	6	7891.285	-0.001
						6	5	7891.510	0.000
						5	4	7891.253	0.002
6	3	3	5	3	2	7	6	7891.710	0.000
						6	5	7891.937	-0.001
						5	4	7891.678	0.002
6	0	6	5	1	5	7	6	6466.002	0.002
						6	5	6466.834	0.000
						5	4	6465.850	-0.002
6	1	6	5	0	5	7	6	9162.339	0.000
						6	5	9161.456	-0.001
						5	4	9162.515	0.000
6	1	5	5	0	5	7	6	9986.337	0.002
						6	5	9987.331	0.000
						5	4	9986.191	-0.002
7	0	7	6	0	6	8	7	9164.321	0.000
						7	6	9164.251	0.000
						6	5	9164.345	0.000
7	0	7	6	1	6	8	7	7865.768	0.002
						7	6	7866.523	0.000
						6	5	7865.649	-0.002
7	1	7	6	0	6	8	7	10354.791	-0.002
						7	6	10353.961	0.000
						6	5	10354.928	0.001
7	1	6	6	0	6	8	7	11452.872	0.000
						7	6	11453.930	-0.002
						6	5	11452.733	-0.001
8	0	8	7	0	7	9	8	10460.588	0.001
						8	7	10460.509	0.001
						7	6	10460.608	0.001

Table S5. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer GG of norephedrine.

$J'$	$K'_{-1}$	$K'_{+1}$	$J''$	$K''_{-1}$	$K''_{+1}$	$F'$	$F''$	$\nu_{obs}$	$\nu_{obs} - \nu_{cal}$
4	0	4	3	0	3	5	4	5956.114	-0.001
						4	3	5955.984	-0.002
						3	2	5956.174	-0.003
4	1	4	3	0	3	5	4	6708.913	0.000
						4	3	6708.006	-0.002
						3	2	6709.175	0.000
4	1	3	3	0	3	5	4	7525.923	0.005
						4	3	7526.909	0.004
						3	2	7525.695	0.001
5	0	5	4	0	4	6	5	7414.010	0.001
						5	4	7413.854	0.001
						4	3	7414.052	-0.002
5	1	5	4	0	4	6	5	8030.698	-0.001
						5	4	8029.905	-0.001
						4	3	8030.874	0.000
5	1	4	4	0	4	6	5	9253.696	0.002
						5	4	9254.809	0.000
						4	3	9253.483	0.002
6	0	6	5	0	5	7	6	8855.541	0.002
						6	5	8855.370	0.000
						5	4	8855.571	0.000
6	1	6	5	0	5	7	6	9339.947	0.000
						6	5	9339.276	-0.001
						5	4	9340.064	0.000
6	1	5	5	0	5	7	6	11045.386	-0.004
						6	5	11046.622	-0.004
						5	4	11045.184	-0.002
7	0	7	6	0	6	8	7	10282.811	0.003
						7	6	10282.643	0.002
						6	5	10282.831	0.001
7	1	7	6	0	6	8	7	10648.652	-0.001
						7	6	10648.113	0.000
						6	5	10648.728	-0.001

Table S6. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer GA of norephedrine.

$J'$	$K'_{-1}$	$K'_{+1}$	$J''$	$K''_{-1}$	$K''_{+1}$	$F'$	$F''$	$\omega_{bs}$	$\omega_{bs}-\omega_{cal}$
3	1	2	2	0	2	4	3	5729.342	-0.001
						3	2	5728.339	-0.001
4	0	4	3	0	3	5	4	5272.614	0.000
						4	3	5272.705	0.000
						3	2	5272.651	0.001
4	1	4	3	1	3	5	4	5152.530	-0.001
						4	3	5152.635	0.001
						3	2	5152.623	-0.001
4	1	3	3	1	2	5	4	5429.636	0.001
						4	3	5429.701	0.000
						3	2	5429.579	0.002
4	1	3	3	0	3	5	4	7196.476	0.001
						4	3	7195.463	0.002
						3	2	7196.796	-0.001
5	0	5	4	0	4	6	5	6573.887	0.001
						5	4	6573.993	0.002
						4	3	6573.904	0.000
5	1	5	4	1	4	6	5	6436.638	-0.001
						5	4	6436.710	-0.001
						4	3	6436.696	-0.003
5	1	4	4	0	4	6	5	8706.201	0.001
						5	4	8705.144	0.000
						4	3	8706.456	0.001
6	0	6	5	0	5	7	6	7864.869	-0.001
						6	5	7864.987	-0.001
						5	4	7864.879	-0.001
6	1	5	5	0	5	7	6	10263.942	-0.001
						6	5	10262.826	-0.001
						5	4	10264.159	-0.001
7	0	7	6	0	6	8	7	9144.967	-0.001
						7	6	9145.093	-0.001
						6	5	9144.973	0.000
7	1	7	6	1	6	8	7	8997.254	0.000
						7	6	8997.307	0.001
						6	5	8997.283	-0.001
8	0	8	7	0	7	9	8	10414.657	-0.001
						8	7	10414.788	0.001
						7	6	10414.663	0.001
8	1	8	7	1	7	9	8	10273.380	0.001
						8	7	10273.427	0.001
						7	6	10273.401	0.000



Table S7. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer AGa of ephedrine.

$J'$	$K'_{-l}$	$K'_{+l}$	$J''$	$K''_{-l}$	$K''_{+l}$	$F'$	$F''$	<i>vobs</i>	<i>vobs-vcsl</i>
4	1	4	3	0	3	5	4	5456.862	-0.002
						4	3	5456.264	-0.002
						3	2	5457.093	0.000
4	1	3	3	0	3	5	4	5750.463	0.001
						4	3	5750.873	0.002
						3	2	5750.432	-0.001
5	0	5	4	0	4	6	5	5139.830	0.000
						5	4	5139.817	-0.001
						4	3	5139.876	-0.001
						4	4	5138.847	0.000
5	2	3	4	2	2	6	5	5156.205	-0.002
						5	4	5156.408	-0.002
						4	3	5156.186	0.000
5	1	5	4	0	4	6	5	6415.584	-0.001
						5	4	6415.031	0.000
						4	3	6415.741	-0.001
5	1	4	4	0	4	6	5	6856.032	0.001
						5	4	6856.500	0.002
						4	3	6855.978	-0.001
6	0	6	5	0	5	7	6	6163.066	0.000
						6	5	6163.047	0.002
						5	4	6163.102	0.003
						6	6	6163.852	0.001
						5	5	6162.130	0.001
6	1	6	5	1	5	7	6	6086.683	0.000
						6	5	6086.704	0.000
						5	4	6086.690	0.002
6	1	5	5	1	4	7	6	6262.782	0.000
						6	5	6262.812	-0.002
						5	4	6262.821	-0.001
6	2	4	5	2	3	7	6	6191.405	0.003
						5	4	6191.405	0.003
						6	5	6191.540	0.003
6	1	6	5	0	5	7	6	7362.435	-0.002
						6	5	7361.919	0.001
						5	4	7362.555	0.001
6	1	5	5	0	5	7	6	7978.984	0.002
						6	5	7979.495	0.001
						5	4	7978.924	0.000
7	0	7	6	0	6	8	7	7183.807	0.000
						7	6	7183.778	0.000
						6	5	7183.828	-0.002
						7	7	7184.563	0.000
						6	6	7182.912	-0.001
7	1	7	6	1	6	8	7	7099.593	0.000
						7	6	7099.605	0.001
						6	5	7099.599	0.000

Table S7 (cont.). Observed frequencies and residuals (in MHz) for the rotational transitions of conformer AGa of ephedrine.

$J'$	$K'_{-1}$	$K'_{+1}$	$J''$	$K''_{-1}$	$K''_{+1}$	$F'$	$F''$	<i>vobs</i>	<i>vobs-vcal</i>
7	1	6	6	1	5	8	7	7304.800	-0.001
						7	6	7304.817	-0.001
						6	5	7304.831	-0.001
7	2	6	6	2	5	8	7	7204.519	-0.002
						7	6	7204.582	-0.001
						6	5	7204.526	-0.001
7	2	5	6	2	4	8	7	7228.643	-0.001
						6	5	7228.643	-0.001
						7	6	7228.743	0.001
7	0	7	6	1	6	8	7	5984.436	0.000
						7	6	5984.906	0.000
						6	5	5984.376	0.001
7	1	7	6	0	6	8	7	8298.966	0.001
						7	6	8298.474	-0.001
						6	5	8299.052	-0.002
7	1	6	6	0	6	8	7	9120.717	-0.001
						7	6	9121.266	-0.001
						6	5	9120.655	-0.001
8	0	8	7	0	7	9	8	8201.756	0.001
						8	7	8201.722	0.000
						7	6	8201.775	0.001
						7	7	8200.910	0.000
8	1	8	7	1	7	9	8	8111.845	0.001
						8	7	8111.850	0.002
						7	6	8111.850	0.002
8	1	7	7	0	7	9	8	10282.847	0.001
						8	7	10283.432	-0.001
						7	6	10282.787	0.001
8	2	7	7	2	6	9	8	8232.287	0.001
						7	6	8232.292	-0.001
						8	7	8232.324	-0.002
8	1	8	7	0	7	9	8	9227.001	-0.001
						8	7	9226.548	0.003
						7	6	9227.074	0.001
8	0	8	7	1	7	7	6	7086.550	0.000
						9	8	7086.597	-0.001
						8	7	7087.025	0.000
9	0	9	8	1	8	10	9	8191.459	-0.002
						9	8	8191.844	0.000
						8	7	8191.423	0.000

Table S8. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer GGa of ephedrine.

$J'$	$K'_{-l}$	$K'_{+l}$	$J''$	$K''_{-l}$	$K''_{+l}$	$F'$	$F''$	$V_{obs}$	$V_{obs}-V_{cal}$
4	1	4	3	0	3	5	4	5546.022	0.001
						4	3	5545.263	0.001
						3	2	5546.290	0.001
4	1	3	3	0	3	5	4	5745.967	-0.001
						3	2	5745.888	0.000
						4	3	5746.559	0.000
5	0	5	4	0	4	6	5	5818.208	0.000
						5	4	5818.187	0.001
						4	3	5818.254	-0.001
5	1	5	4	1	4	6	5	5772.901	0.004
						4	3	5772.901	0.004
						5	4	5772.935	0.002
5	1	4	4	1	3	6	5	5872.983	0.001
						5	4	5873.039	0.002
						4	3	5873.045	0.000
5	2	4	4	2	3	6	5	5823.571	-0.001
						4	3	5823.553	-0.002
						5	4	5823.742	0.000
5	2	3	4	2	2	6	5	5829.644	-0.002
						4	3	5829.625	0.000
						5	4	5829.849	-0.002
5	1	5	4	0	4	6	5	6662.535	0.000
						5	4	6661.820	0.000
						4	3	6662.720	-0.001
5	1	4	4	0	4	6	5	6962.564	-0.001
						5	4	6963.221	0.000
						4	3	6962.471	-0.001
6	0	6	5	0	5	7	6	6978.537	0.000
						6	5	6978.504	0.001
						5	4	6978.567	-0.001
6	1	6	5	1	5	7	6	6926.675	0.000
						5	4	6926.675	0.000
						6	5	6926.691	0.000
6	1	5	5	1	4	7	6	7046.698	0.000
						6	5	7046.728	0.001
						5	4	7046.744	0.002
6	2	5	5	2	4	7	6	6987.742	-0.001
						5	4	6987.742	-0.001
						6	5	6987.839	0.000
6	2	4	5	2	3	7	6	6998.334	-0.001
						5	4	6998.334	-0.001
						6	5	6998.473	-0.003
6	0	6	5	1	5	7	6	6134.212	0.001
						6	5	6134.868	-0.001
						5	4	6134.102	0.001
6	1	6	5	0	5	7	6	7771.001	-0.001
						6	5	7770.325	0.000
						5	4	7771.141	-0.001

Table S8 (cont.). Observed frequencies and residuals (in MHz) for the rotational transitions of conformer GGa of ephedrine.

$J'$	$K'_{-1}$	$K'_{+1}$	$J''$	$K''_{-1}$	$K''_{+1}$	$F'$	$F''$	$V_{obs}$	$V_{obs}-V_{cal}$
6	1	5	5	0	5	7	6	8191.053	-0.001
						6	5	8191.762	0.000
						5	4	8190.960	0.000
7	0	7	6	0	6	8	7	8137.116	-0.001
						7	6	8137.074	0.000
						6	5	8137.145	0.004
7	1	7	6	1	6	8	7	8080.033	0.000
						6	5	8080.033	0.000
7	1	6	6	1	5	8	7	8219.892	0.000
						7	6	8219.907	0.001
						6	5	8219.927	0.000
7	2	6	6	2	5	8	7	8151.590	-0.001
						7	6	8151.652	0.001
						6	5	8151.599	0.001
7	2	5	6	2	4	8	7	8168.440	-0.004
						6	5	8168.440	-0.004
						7	6	8168.550	0.000
7	0	7	6	1	6	8	7	7344.649	-0.003
						7	6	7345.251	-0.001
						6	5	7344.566	-0.001
7	1	7	6	0	6	8	7	8872.499	0.000
						7	6	8871.854	-0.004
						6	5	8872.601	-0.005
7	1	6	6	0	6	8	7	9432.412	0.002
						7	6	9433.167	0.001
						6	5	9432.320	0.001
8	0	8	7	0	7	9	8	9293.745	-0.001
						8	7	9293.695	-0.002
						7	6	9293.765	0.000
8	1	8	7	1	7	9	8	9232.924	-0.001
						8	7	9232.929	0.004
						7	6	9232.935	0.005
8	1	7	7	1	6	9	8	9392.461	0.003
						8	7	9392.465	0.003
						7	6	9392.486	0.001
8	2	7	7	2	6	9	8	9315.074	0.001
						8	7	9315.111	0.002
						7	6	9315.083	0.003
8	2	6	7	2	5	9	8	9340.118	-0.003
						7	6	9340.118	-0.003
						8	7	9340.209	-0.001
8	0	8	7	1	7	9	8	8558.364	-0.001
						8	7	8558.915	0.002
						7	6	8558.306	0.005
8	1	8	7	0	7	9	8	9968.307	0.000
						8	7	9967.710	0.001
						7	6	9968.396	0.001
9	0	9	8	1	8	10	9	9773.726	-0.003
						9	8	9774.218	-0.003
						8	7	9773.670	-0.004

Table S9. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer AGb of ephedrine.

$J'$	$K'_{-l}$	$K'_{+l}$	$J''$	$K''_{-l}$	$K''_{+l}$	$F'$	$F''$	$V_{obs}$	$V_{obs}-V_{cal}$
4	1	4	3	0	3	5	4	5400.374	0.001
						4	3	5399.156	-0.001
						3	2	5400.761	0.000
5	1	5	4	0	4	6	5	6309.942	-0.001
						5	4	6308.773	-0.001
						4	3	6310.223	0.000
6	0	6	5	0	5	7	6	5860.651	0.000
						6	5	5860.598	0.000
						5	4	5860.685	0.000
6	1	6	5	1	5	7	6	5784.992	-0.001
						6	5	5785.001	0.001
						5	4	5784.980	0.002
6	1	5	5	1	4	7	6	5956.519	0.000
						6	5	5956.549	-0.001
						5	4	5956.582	0.001
6	2	5	5	2	4	7	6	5872.057	-0.001
						5	4	5872.057	-0.001
						6	5	5872.154	0.001
6	2	4	5	2	3	7	6	5885.187	0.003
						5	4	5885.187	0.003
						6	5	5885.348	0.000
6	1	6	5	0	5	7	6	7207.638	-0.001
						6	5	7206.514	-0.001
						5	4	7207.855	0.000
7	0	7	6	0	6	8	7	6831.824	0.001
						7	6	6831.761	0.000
						6	5	6831.852	-0.001
7	1	7	6	1	6	8	7	6747.815	0.000
						7	6	6747.810	-0.001
						6	5	6747.804	-0.002
7	1	6	6	1	5	8	7	6947.750	0.000
						7	6	6947.764	0.001
						6	5	6947.799	0.002
7	2	6	6	2	5	8	7	6849.793	0.001
						7	6	6849.850	-0.001
						6	5	6849.802	0.004
7	2	5	6	2	4	8	7	6870.707	0.001
						6	5	6870.707	0.001
						7	6	6870.836	0.000
7	0	7	6	1	6	8	7	5484.836	0.000
						7	6	5485.842	-0.001
						6	5	5484.684	0.000
7	1	7	6	0	6	8	7	8094.801	-0.002
						7	6	8093.727	-0.001
						6	5	8094.975	0.000
8	0	8	7	0	7	9	8	7800.532	-0.001
						8	7	7800.455	-0.001
						7	6	7800.552	-0.001

Table S9 (cont.). Observed frequencies and residuals (in MHz) for the rotational transitions of conformer AGb of ephedrine.

$J'$	$K'_{-l}$	$K'_{+l}$	$J''$	$K''_{-l}$	$K''_{+l}$	$F'$	$F''$	$V_{obs}$	$V_{obs}-V_{cal}$
8	1	8	7	1	7	9	8	7710.057	0.000
						8	7	7710.045	-0.001
8	1	7	7	1	6	9	8	7938.227	0.000
						8	7	7938.227	0.000
						7	6	7938.262	0.000
8	2	7	7	2	6	9	8	7827.079	0.001
						8	7	7827.113	0.002
						7	6	7827.087	0.002
8	2	6	7	2	5	9	8	7858.235	-0.001
						7	6	7858.235	-0.001
						8	7	7858.351	0.001
8	0	8	7	1	7	9	8	6537.554	-0.001
8	0	8	7	1	7	8	7	6538.489	0.000
						7	6	6537.430	-0.001
8	1	8	7	0	7	9	8	8973.035	0.000
						8	7	8972.017	0.003
						7	6	8973.170	-0.003
9	0	9	8	0	8	10	9	8766.564	-0.001
						9	8	8766.479	-0.001
						8	7	8766.582	0.000
9	1	9	8	1	8	10	9	8671.665	0.003
						8	7	8671.665	0.003
						9	8	8671.649	0.000
9	1	8	8	1	7	10	9	8927.807	-0.001
						9	8	8927.797	-0.002
						8	7	8927.835	-0.002
9	2	8	8	2	7	10	9	8803.856	0.001
						8	7	8803.865	0.002
						9	8	8803.876	0.002
9	0	9	8	1	8	10	9	7594.062	-0.001
						9	8	7594.921	-0.001
						8	7	7593.960	-0.001
9	1	9	8	0	8	10	9	9844.166	-0.001
						9	8	9843.205	-0.001
						8	7	9844.282	0.002

Table S10. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer AGa of pseudoephedrine.

$J'$	$K'_{-1}$	$K'_{+1}$	$J''$	$K''_{-1}$	$K''_{+1}$	$F'$	$F''$	$\nu_{obs}$	$\nu_{obs}-\nu_{cal}$
3	2	2	2	1	2	4	3	7567.668	-0.004
						3	2	7568.247	-0.003
						2	1	7567.343	-0.005
3	2	1	2	1	1	4	3	7471.960	-0.002
						3	2	7470.564	-0.003
						2	1	7472.751	0.001
4	1	4	3	0	3	5	4	5299.657	0.001
						4	3	5298.500	0.001
						3	2	5300.034	0.000
5	1	5	4	0	4	6	5	6205.912	0.001
						5	4	6204.811	0.001
						4	3	6206.181	0.002
5	1	4	4	0	4	6	5	6699.256	0.001
						5	4	6700.342	0.001
						4	3	6699.080	0.002
6	0	6	5	0	5	7	6	5894.715	-0.002
						6	5	5894.651	-0.002
						5	4	5894.750	-0.002
6	1	6	5	1	5	7	6	5810.327	-0.002
						6	5	5810.337	0.001
						5	4	5810.316	-0.001
6	1	5	5	1	4	7	6	6007.642	0.000
						6	5	6007.670	-0.002
						5	4	6007.703	-0.001
6	1	6	5	0	5	7	6	7099.158	0.000
						6	5	7098.111	0.001
						5	4	7099.364	0.001
6	1	5	5	0	5	7	6	7789.817	0.001
						6	5	7790.981	0.003
						5	4	7789.650	0.003
7	0	7	6	0	6	8	7	6869.321	-0.001
						7	6	6869.248	-0.001
						6	5	6869.354	0.000
7	1	7	6	1	6	8	7	6776.844	0.001
						7	6	6776.837	-0.001
						6	5	6776.837	-0.001
7	1	6	6	1	5	8	7	7006.724	-0.001
						7	6	7006.735	0.000
						6	5	7006.770	-0.001
7	1	7	6	0	6	8	7	7981.287	0.002
						7	6	7980.298	0.002
						6	5	7981.451	0.003
7	1	6	6	0	6	8	7	8901.830	0.006
						7	6	8903.058	-0.001
						6	5	8901.669	0.003
8	0	8	7	0	7	9	8	7840.565	0.000
						8	7	7840.477	-0.001
						7	6	7840.586	-0.001
8	1	8	7	1	7	9	8	7742.564	0.003
						7	6	7742.564	0.003
						8	7	7742.549	-0.003

Table S10 (cont.). Observed frequencies and residuals (in MHz) for the rotational transitions of conformerAGa of pseudoephedrine.

$J'$	$K'_{-l}$	$K'_{+l}$	$J''$	$K''_{-l}$	$K''_{+l}$	$F'$	$F''$	$\nu_{obs}$	$\nu_{obs}-\nu_{cal}$
8	1	7	7	1	6	9	8	8004.709	0.002
						8	7	8004.709	0.002
						7	6	8004.744	0.000
8	0	8	7	1	7	9	8	6728.598	-0.004
						8	7	6729.425	-0.005
						7	6	6728.489	-0.004
9	0	9	8	0	8	10	9	8808.241	0.000
						9	8	8808.146	0.000
						8	7	8808.260	0.001



Table S11. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer GGb of pseudoephedrine.

$J'$	$K'_{-1}$	$K'_{+1}$	$J''$	$K''_{-1}$	$K''_{+1}$	$F'$	$F''$	$\nu_{obs}$	$\nu_{obs}-\nu_{cal}$
4	1	4	3	0	3	5	4	5725.922	0.003
						4	3	5726.107	0.005
						3	2	5725.937	0.002
5	0	5	4	0	4	6	5	5944.053	0.002
						5	4	5944.073	0.002
5	1	5	4	0	4	6	5	6878.189	0.000
						5	4	6878.398	-0.001
6	0	6	5	0	5	7	6	7131.027	-0.001
						6	5	7131.050	0.002
6	1	6	5	1	5	7	6	7089.769	-0.001
						6	5	7089.801	-0.002
6	1	6	5	0	5	7	6	8023.904	-0.005
						6	5	8024.126	-0.004
7	0	7	6	0	6	8	7	8317.022	0.001
						7	6	8317.043	0.001
						6	5	8317.037	0.000
7	1	6	6	1	5	8	7	8377.463	-0.004
						7	6	8377.484	-0.003
8	0	8	7	0	7	9	8	9501.892	-0.001
						8	7	9501.915	0.001
8	1	8	7	1	7	9	8	9451.539	0.003
						8	7	9451.559	0.004

Table S12. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer GGa of pseudoephedrine.

$J'$	$K'_{-l}$	$K'_{+l}$	$J''$	$K''_{-l}$	$K''_{+l}$	$F'$	$F''$	$\nu_{obs}$	$\nu_{obs} - \nu_{cal}$
3	2	2	2	1	2	4	3	6628.791	0.000
3	2	1	2	1	1	4	3	6564.227	-0.005
4	1	4	3	0	3	5	4	5404.364	-0.004
						4	3	5404.421	-0.003
						3	2	5404.398	0.002
5	1	5	4	0	4	6	5	6456.227	-0.002
						5	4	6456.298	-0.005
						6	5	6787.107	0.009
5	1	4	4	0	4	5	4	6786.934	0.003
						4	3	6787.157	0.000
6	1	6	5	0	5	7	6	7499.222	-0.001
						5	4	7499.222	-0.001
						6	5	7499.303	-0.001
7	1	7	6	0	6	8	7	8534.527	0.004
						6	5	8534.527	0.004
						7	6	8534.614	0.006
8	0	8	7	1	7	9	8	7996.216	-0.005
						8	7	7996.157	-0.004
						7	6	7996.241	0.002

Table S13. Observed frequencies and residuals (in MHz) for the rotational transitions of conformerAGb of pseudoephedrine.

$J'$	$K'_{-l}$	$K'_{+l}$	$J''$	$K''_{-l}$	$K''_{+l}$	$F'$	$F''$	$\nu_{obs}$	$\nu_{obs}-\nu_{cal}$
3	2	2	2	1	2	2	1	7783.409	0.000
						4	3	7783.672	0.001
						3	2	7784.141	0.001
3	2	1	2	1	1	3	2	7656.775	-0.001
						4	3	7658.033	-0.002
						2	1	7658.746	-0.002
5	1	5	4	0	4	6	5	6309.793	0.000
						5	4	6308.833	0.000
						4	3	6310.031	0.000
5	1	4	4	0	4	6	5	6961.782	-0.001
						5	4	6962.752	0.000
6	0	6	5	0	5	7	6	6052.110	-0.001
						6	5	6052.038	-0.001
						5	4	6052.146	-0.001
6	1	6	5	1	5	7	6	5946.022	-0.001
						6	5	5946.029	0.000
						5	4	5946.014	-0.002
6	1	6	5	0	5	7	6	7204.279	0.000
						6	5	7203.379	-0.001
						5	4	7204.458	0.001
6	1	5	5	0	5	5	4	8116.578	0.002
						7	6	8116.728	0.002
7	0	7	6	0	6	8	7	7047.731	0.001
						7	6	7047.648	0.001
						6	5	7047.761	0.000
7	1	7	6	1	6	8	7	6933.919	0.002
						7	6	6933.919	0.002
						6	5	6933.919	0.002
7	1	6	6	1	5	8	7	7237.080	0.002
						7	6	7237.080	0.002
						6	5	7237.117	-0.001
7	1	7	6	0	6	8	7	8086.086	-0.001
						7	6	8085.254	0.000
						6	5	8086.230	0.003
8	0	8	7	0	7	9	8	8038.017	0.001
						8	7	8037.922	0.000
						7	6	8038.038	-0.001
8	1	8	7	1	7	9	8	7920.533	0.000
						7	6	7920.533	0.000
						8	7	7920.520	0.000
8	1	7	7	1	6	9	8	8265.729	0.000
						8	7	8265.719	-0.001
						7	6	8265.761	-0.002
8	0	8	7	1	7	9	8	6999.658	-0.001
						8	7	7000.313	0.000
						7	6	6999.574	0.001
9	0	9	8	0	8	10	9	9022.907	0.000
						9	8	9022.806	0.001
						8	7	9022.925	0.000

Table S13 (cont.). Observed frequencies and residuals (in MHz) for the rotational transitions of conformer AGb of pseudoephedrine.

$J'$	$K'_{-j}$	$K'_{+j}$	$J''$	$K''_{-j}$	$K''_{+j}$	$F'$	$F''$	$\nu_{obs}$	$\nu_{obs} - \nu_{cal}$
9	1	9	8	1	8	10	9	8905.789	0.001
						8	7	8905.789	0.001
						9	8	8905.770	0.001
9	1	8	8	1	7	10	9	9292.042	-0.001
						9	8	9292.022	-0.001
						8	7	9292.069	-0.002

Table S14. Predicted ab initio structure of the AG conformer of norephedrine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.533538	-1.257858	-0.178641
2	6	0	-3.184829	-0.118840	0.312226
3	6	0	-2.487800	1.091916	0.405213
4	6	0	-1.140507	1.164784	0.029519
5	6	0	-0.482296	0.024895	-0.452781
6	6	0	-1.189088	-1.183279	-0.558818
7	6	0	0.985041	0.053717	-0.791780
8	6	0	1.828358	-0.638214	0.302462
9	7	0	3.235061	-0.463049	-0.095633
10	8	0	1.421887	1.390086	-0.960059
11	6	0	1.616880	-0.017760	1.677441
12	1	0	-4.230249	-0.171806	0.604446
13	1	0	-2.993195	1.981925	0.771839
14	1	0	-0.592910	2.099676	0.094832
15	1	0	-0.689986	-2.065808	-0.956516
16	1	0	-3.071113	-2.198375	-0.268614
17	1	0	1.140378	-0.510121	-1.728321
18	1	0	2.385633	1.330414	-0.864372
19	1	0	1.526486	-1.696090	0.335145
20	1	0	2.269253	-0.500375	2.413706
21	1	0	0.581691	-0.144489	2.003193
22	1	0	1.847822	1.050937	1.653026
23	1	0	3.856745	-0.677033	0.678633
24	1	0	3.475603	-1.094370	-0.856152
Rotational constants (GHZ):			2.3232607	0.6834601	0.6442475

Table S15. Predicted ab initio structure of the GG conformer of norephedrine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.467907	1.073129	-0.331981
2	6	0	3.003636	0.029410	0.432699
3	6	0	2.216697	-1.092900	0.719138
4	6	0	0.895019	-1.164306	0.261383
5	6	0	0.342065	-0.112509	-0.486347
6	6	0	1.146158	0.998955	-0.785902
7	6	0	-1.105634	-0.141693	-0.931988
8	6	0	-2.050812	0.409845	0.158133
9	7	0	-2.075600	-0.576901	1.247866
10	8	0	-1.543113	-1.440936	-1.291496
11	6	0	-1.708172	1.830237	0.597547
12	1	0	4.031085	0.080330	0.783040
13	1	0	2.633718	-1.917046	1.292565
14	1	0	0.300687	-2.051160	0.461573
15	1	0	0.737526	1.805683	-1.392197
16	1	0	3.078937	1.937217	-0.580381
17	1	0	-1.207757	0.489155	-1.823331
18	1	0	-1.855791	-1.822478	-0.456259
19	1	0	-3.051430	0.397733	-0.291486
20	1	0	-0.732415	1.857834	1.093280
21	1	0	-1.674803	2.510634	-0.261007
22	1	0	-2.463729	2.201259	1.297781
23	1	0	-1.263482	-0.455581	1.849605
24	1	0	-2.899606	-0.448784	1.827630
Rotational constants (GHZ):			1.8511703	0.7955204	0.7179294

Table S16. Predicted ab initio structure of the GA conformer of norephedrine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.567471	-0.940055	0.706382
2	6	0	3.170043	-0.168828	-0.294850
3	6	0	2.416592	0.793621	-0.980656
4	6	0	1.062214	0.971455	-0.677861
5	6	0	0.451983	0.203034	0.328603
6	6	0	1.213716	-0.755032	1.014289
7	6	0	-1.022321	0.365377	0.612497
8	6	0	-1.872266	-0.268378	-0.493503
9	7	0	-1.491179	-1.680161	-0.600514
10	8	0	-1.402290	1.742512	0.675055
11	6	0	-3.357014	-0.177696	-0.165709
12	1	0	4.221411	-0.308367	-0.531923
13	1	0	2.881553	1.396795	-1.756369
14	1	0	0.475077	1.721591	-1.202465
15	1	0	0.740061	-1.358081	1.786014
16	1	0	3.148882	-1.683481	1.245628
17	1	0	-1.266679	-0.146661	1.555093
18	1	0	-0.808364	2.165367	1.304096
19	1	0	-1.669267	0.304066	-1.414001
20	1	0	-3.952897	-0.612705	-0.975855
21	1	0	-3.658496	0.862676	-0.031297
22	1	0	-3.565354	-0.736746	0.752512
23	1	0	-2.120032	-2.154149	-1.243305
24	1	0	-0.551828	-1.770266	-0.980120
Rotational constants (GHZ):			2.1989485	0.6996793	0.6341399

Table S17. Predicted ab initio structure of the AGa conformer of ephedrine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.964016	-0.963148	0.011168
2	6	0	1.604369	-1.098029	-0.296939
3	6	0	0.794913	0.039672	-0.419817
4	6	0	1.363262	1.310355	-0.238049
5	6	0	2.720034	1.445434	0.075902
6	6	0	3.523300	0.305256	0.208517
7	1	0	3.586821	-1.850032	0.098232
8	1	0	1.161992	-2.076641	-0.454895
9	6	0	-0.684521	-0.074310	-0.678319
10	1	0	0.744453	2.198583	-0.357726
11	1	0	3.149276	2.434849	0.212093
12	1	0	4.578641	0.406389	0.447600
13	6	0	-1.500620	0.211906	0.606028
14	6	0	-1.053423	-0.657558	1.775677
15	8	0	-1.006074	-1.366958	-1.159549
16	7	0	-2.905815	-0.075575	0.296326
17	1	0	-3.409455	-0.232722	1.164036
18	1	0	-1.119111	-1.716927	1.511074
19	1	0	-1.690798	-0.472706	2.647873
20	1	0	-0.021220	-0.432323	2.053670
21	1	0	-1.946981	-1.462907	-0.935286
22	1	0	-0.959149	0.682174	-1.430600
23	1	0	-1.356577	1.276107	0.864771
24	6	0	-3.574443	0.977000	-0.471798
25	1	0	-3.447446	1.976546	-0.027139
26	1	0	-4.641860	0.751560	-0.534650
27	1	0	-3.180621	1.003279	-1.491156
Rotational constants (GHZ):			2.0143906	0.5327766	0.5045588



Table S18. Predicted ab initio structure of the GGa conformer of ephedrine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.336619	-1.370248	-0.632752
2	6	0	-1.119094	-1.207801	0.040293
3	6	0	-0.756475	0.042493	0.566311
4	6	0	-1.649615	1.117292	0.429722
5	6	0	-2.868228	0.958551	-0.240037
6	6	0	-3.210389	-0.286255	-0.782819
7	1	0	-2.606698	-2.345261	-1.030823
8	1	0	-0.460394	-2.060149	0.180642
9	6	0	0.587617	0.254017	1.232318
10	1	0	-1.393065	2.082876	0.862431
11	1	0	-3.551157	1.799567	-0.329886
12	1	0	-4.157853	-0.415355	-1.299216
13	6	0	1.685940	0.605174	0.202700
14	6	0	1.356907	1.833352	-0.643477
15	8	0	1.016748	-0.874524	1.974111
16	7	0	1.962877	-0.612817	-0.567956
17	1	0	1.233800	-0.728941	-1.269713
18	1	0	0.482191	1.644944	-1.274625
19	1	0	2.201295	2.099632	-1.286484
20	1	0	1.136947	2.696785	-0.005575
21	1	0	1.488546	-1.410105	1.315092
22	1	0	0.499478	1.089888	1.937172
23	1	0	2.589883	0.801013	0.795486
24	6	0	3.274288	-0.620930	-1.218387
25	1	0	3.439985	0.223827	-1.902772
26	1	0	3.386615	-1.549364	-1.784201
27	1	0	4.050303	-0.597317	-0.447956
Rotational constants (GHZ):			1.5657045	0.5970831	0.5793337

Table S19. Predicted ab initio structure of the AGb conformer of ephedrine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.955704	0.854854	0.626952
2	6	0	-1.641646	1.109702	0.214405
3	6	0	-0.908376	0.116963	-0.450289
4	6	0	-1.506527	-1.128190	-0.699927
5	6	0	-2.817237	-1.384966	-0.283445
6	6	0	-3.543443	-0.393418	0.389026
7	1	0	-3.520172	1.631951	1.136308
8	1	0	-1.178564	2.075282	0.391532
9	6	0	0.528158	0.337376	-0.846247
10	1	0	-0.949738	-1.894915	-1.236826
11	1	0	-3.270500	-2.352217	-0.485030
12	1	0	-4.563262	-0.587799	0.710395
13	6	0	1.501003	-0.416329	0.086016
14	6	0	1.340810	0.003365	1.542674
15	8	0	0.828930	1.722782	-0.838163
16	7	0	2.848544	-0.098123	-0.410087
17	1	0	2.911495	-0.449424	-1.364260
18	1	0	1.988827	-0.585924	2.196648
19	1	0	0.307744	-0.156018	1.862594
20	1	0	1.584838	1.062751	1.665605
21	1	0	1.797363	1.748854	-0.791757
22	1	0	0.674338	-0.068521	-1.863417
23	1	0	1.281111	-1.496107	0.001227
24	6	0	3.943172	-0.688246	0.364398
25	1	0	4.056425	-0.161860	1.313770
26	1	0	4.873459	-0.568617	-0.196534
27	1	0	3.794128	-1.759497	0.574279
Rotational constants (GHZ):			2.1121478	0.5072078	0.4800149

Table S20. Predicted ab initio structure of the AGa conformer of pseudoephedrine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.394419	-1.058139	-0.584684
2	6	0	2.703595	-0.911039	-1.055627
3	6	0	3.520388	0.113970	-0.559505
4	6	0	3.029215	0.977596	0.426895
5	6	0	1.720754	0.824036	0.901500
6	6	0	0.892921	-0.188303	0.396118
7	1	0	0.762801	-1.864267	-0.948295
8	1	0	3.086864	-1.593840	-1.809781
9	1	0	4.537363	0.226903	-0.925763
10	1	0	3.663351	1.763792	0.828668
11	1	0	1.342169	1.488162	1.676541
12	6	0	-0.539070	-0.308770	0.842263
13	1	0	-0.671759	0.264310	1.777369
14	6	0	-1.506634	0.272023	-0.206198
15	8	0	-0.853295	-1.675352	1.055217
16	1	0	-1.824381	-1.683838	1.014231
17	7	0	-2.868473	-0.050593	0.247130
18	6	0	-1.264582	1.758858	-0.460465
19	1	0	-1.345013	-0.297609	-1.131804
20	6	0	-3.866475	-0.044796	-0.824535
21	1	0	-3.138943	0.622764	0.962310
22	1	0	-3.914256	0.900160	-1.385339
23	1	0	-3.633198	-0.850029	-1.526678
24	1	0	-4.852743	-0.242860	-0.397097
25	1	0	-2.009688	2.162019	-1.153181
26	1	0	-1.331422	2.318786	0.480748
27	1	0	-0.272652	1.929891	-0.888141
Rotational constants (GHZ):			1.9967356	0.5127097	0.4816769

Table S21. Predicted ab initio structure of the GGa conformer of pseudoephedrine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.473150	-0.417349	-1.088234
2	6	0	2.743891	0.171694	-1.147355
3	6	0	3.363937	0.631380	0.019712
4	6	0	2.715161	0.483497	1.253213
5	6	0	1.445905	-0.101129	1.308794
6	6	0	0.811204	-0.554723	0.139779
7	1	0	1.001866	-0.796702	-1.990061
8	1	0	3.248634	0.268225	-2.105403
9	1	0	4.350361	1.084918	-0.027232
10	1	0	3.196495	0.822182	2.167188
11	1	0	0.950547	-0.222924	2.271084
12	6	0	-0.595163	-1.122182	0.230093
13	1	0	-0.623324	-1.871493	1.030777
14	6	0	-1.596864	0.001781	0.570443
15	8	0	-1.005430	-1.776069	-0.957665
16	1	0	-1.363632	-1.060680	-1.506518
17	7	0	-1.621370	0.885977	-0.600168
18	6	0	-2.983213	-0.564653	0.860260
19	6	0	-2.555089	2.008358	-0.495396
20	1	0	-0.681389	1.261348	-0.718647
21	1	0	-2.355103	2.707802	-1.310942
22	1	0	-3.582755	1.655492	-0.603662
23	1	0	-2.470902	2.550511	0.460357
24	1	0	-3.670136	0.214277	1.201520
25	1	0	-3.400166	-1.036958	-0.033350
26	1	0	-2.912826	-1.319167	1.649875
27	1	0	-1.232154	0.529833	1.469663
Rotational constants (GHZ):			1.6415410	0.5697097	0.5479362

Table S22. Predicted ab initio structure of the GGb conformer of pseudoephedrine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.612187	-0.601878	0.182630
2	6	0	1.350439	-0.669488	-1.006323
3	6	0	2.675732	-0.215509	-1.045001
4	6	0	3.279464	0.302068	0.106695
5	6	0	2.556479	0.345787	1.306677
6	6	0	1.232380	-0.103171	1.340561
7	6	0	-0.847298	-1.017374	0.235585
8	8	0	-1.283834	-1.641695	-0.955810
9	6	0	-1.771954	0.192325	0.525490
10	6	0	-3.172039	-0.286022	0.898807
11	7	0	-1.834510	1.011340	-0.693394
12	6	0	-0.896124	2.140562	-0.719612
13	1	0	0.885310	-1.086118	-1.894436
14	1	0	3.237357	-0.271557	-1.974299
15	1	0	4.307674	0.652763	0.075515
16	1	0	3.023046	0.727531	2.211414
17	1	0	0.679150	-0.071968	2.278271
18	1	0	-0.972812	-1.749880	1.043244
19	1	0	-1.523426	-0.886804	-1.521058
20	1	0	-2.778616	1.370717	-0.798388
21	1	0	-0.991996	2.789848	0.164605
22	1	0	0.129331	1.770791	-0.763430
23	1	0	-1.082905	2.736275	-1.617314
24	1	0	-3.826585	0.566385	1.111159
25	1	0	-3.602884	-0.870373	0.080671
26	1	0	-3.136243	-0.919467	1.789921
27	1	0	-1.349750	0.772244	1.361309
Rotational constants (GHZ):			1.6382791	0.6158390	0.5953208

Table S23. Predicted ab initio structure of the AGb conformer of pseudoephedrine.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.534500	1.075479	0.489575
2	6	0	2.889211	0.856466	0.762184
3	6	0	3.547474	-0.254421	0.217689
4	6	0	2.849768	-1.133650	-0.619199
5	6	0	1.495603	-0.908609	-0.895326
6	6	0	0.826861	0.190815	-0.338762
7	1	0	1.023443	1.947318	0.889245
8	1	0	3.431751	1.550859	1.398851
9	1	0	4.600054	-0.422950	0.429393
10	1	0	3.358661	-1.987640	-1.058977
11	1	0	0.955616	-1.585508	-1.555183
12	6	0	-0.647100	0.392744	-0.569698
13	1	0	-0.950018	-0.215215	-1.438542
14	6	0	-1.467664	-0.061287	0.655386
15	8	0	-0.909249	1.764509	-0.817089
16	1	0	-1.837924	1.864580	-0.545425
17	7	0	-2.857141	0.382847	0.444939
18	6	0	-1.285165	-1.548830	0.958323
19	1	0	-1.094317	0.525743	1.504962
20	6	0	-3.665921	-0.467721	-0.432124
21	1	0	-3.316658	0.475739	1.345571
22	1	0	-4.658393	-0.021145	-0.531672
23	1	0	-3.215533	-0.498977	-1.427940
24	1	0	-3.782369	-1.499504	-0.073412
25	1	0	-1.953830	-1.859718	1.768618
26	1	0	-1.496880	-2.169073	0.081022
27	1	0	-0.255029	-1.746416	1.267337
Rotational constants (GHZ):			2.0474808	0.5326987	0.4896228