Supplementary Information to

Fingerprint region of the formic acid dimer: variational vibrational computations in curvilinear coordinates

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TABLE I. Normal coordinate definition of FAD corresponding to the QB16-PES: equilibrium structure, $c_{i\alpha}$ in bohr with $i = 1(\mathrm{H}^{(A)}), 2(\mathrm{H}^{(A)}), 5(\mathrm{O}^{(A)}), 6(\mathrm{O}^{(A)}), 9(\mathrm{C}^{(A)}), 3(\mathrm{H}^{(B)}), 4(\mathrm{H}^{(B)}), 7(\mathrm{O}^{(B)}), 8(\mathrm{O}^{(B)}), 10(\mathrm{C}^{(B)})$ and $\alpha = x, y, z$, and $l_{\alpha i,j}$ elements used to calculate the Q_j dimensionless normal coordinates ($j = 1, \ldots, 24$). The harmonic frequencies, $\tilde{\nu}^{\mathrm{HO}}$ in cm^{-1}, are also given in the table. $r_{i\alpha} = c_{i\alpha} + \sum_{j=1}^{24} Q_j l_{\alpha i,j}$

		Q_1	Q_2	Q_3	Q_4	Q_5	Q_6	Q_7	Q_8
$\tilde{\nu}^{\mathrm{HO}}$		70.079	169.973	170.393	208.841	253.821	275.148	692.643	715.565
	$l_{\alpha_i,j}$:								
c_{1x}	0.2868654398	0	−0.0550489068	0	−0.0221897688	0	0.1027336927	0.0106811053	0.0078803994
c_{1y}	0	0.0888640999	0	−0.3653231756	0	−0.2807202366	0	0	0
c_{1z}	−5.6564792624	0	0.0195732544	0	−0.0809832850	0	0.0110746966	−0.0364919882	−0.0370286239
c_{2x}	−2.1440160385	0	0.0678179381	0	0.0208023614	0	−0.0608445441	0.1078648560	0.0925684085
c_{2y}	0	0.0306454227	0	0.1749988335	0	0.0906722954	0	0	0
c_{2z}	−0.8915699548	0	0.1081730397	0	−0.0595051283	0	−0.0790462710	0.0205304089	0.0182074288
c_{5x}	−2.1349725967	0	0.0508401068	0	0.01271590328	0	−0.0029861332	0.0369000130	0.0364542139
c_{5y}	0	0.1530793141	0	0.0551154157	0	0.0477433605	0	0	0
c_{5z}	−2.7675548795	0	0.1027221555	0	−0.0512142095	0	−0.0756204105	0.0175902254	0.0155037351
c_{6x}	2.1002784911	0	0.0706620794	0	0.0178761714	0	−0.0029895689	−0.0407039395	−0.0425354587
c_{6y}	0	−0.1715444148	0	0.0324005323	0	0.0615425686	0	0	0
c_{6z}	−2.2930907605	0	−0.0503750205	0	−0.0967866341	0	0.0748243895	0.0136926724	0.0136488812
c_{9x}	0.2020375225	0	0.0182073300	0	0.0111036095	0	0.0279448602	−0.0002598622	−0.0003293917
c_{9y}	0	0.0156158809	0	−0.1007967531	0	−0.06613055556	0	0	0
c_{9z}	−3.5929593001	0	0.0223423640	0	−0.0795590666	0	0.0067828274	−0.0376791855	−0.0372458161
c_{3x}	−0.2868649484	0	0.0550477261	0	0.0221796487	0	0.1027432996	−0.0106806258	0.0078747894
c_{3y}	0	0.0881415843	0	−0.3655592754	0	0.2804082358	0	0	0
c_{3z}	5.6564793125	0	−0.0195862102	0	0.0809913977	0	−0.0110710456	0.0364889326	−0.0370303283
c_{4x}	2.1440156985	0	−0.0678024450	0	−0.0208138591	0	−0.0608542506	0.1078602975	0.0925736468
c_{4y}	0	0.0306891267	0	0.1751452961	0	−0.0905441001	0	0	0
c_{4z}	0.8915695806	0	−0.1081715038	0	0.0595137351	0	−0.0790584397	−0.0205293799	0.0182076727
c_{7x}	2.1349725840	0	−0.0508269012	0	−0.0127196509	0	−0.0029895689	−0.0368983293	0.0364558854
c_{7y}	0	0.1528925491	0	0.0552385319	0	−0.0477007959	0	0	0
c_{7z}	2.7675545069	0	−0.1027219292	0	0.0512231448	0	−0.0756320465	−0.0175891492	0.0155038045
c_{8x}	−2.1002785866	0	−0.0706452307	0	−0.0178800062	0	−0.0206223309	0.0407027015	−0.0425372096
c_{8y}	0	−0.1720339853	0	0.0325403496	0	−0.0615074767	0	0	0
c_{8z}	2.2930911271	0	0.0503506096	0	0.0967988803	0	0.0748289406	−0.0136918211	0.0136503538
c_{10x}	−0.2020373912	0	−0.0181990479	0	−0.0111065313	0	0.0279449116	0.0002605854	−0.0003293482
c_{10y}	0	0.0151332334	0	0.1007865686	0	−0.0660394431	0	0	0
c_{10z}	3.5929593354	0	−0.0223551486	0	0.0795697925	0	0.0067792673	0.0376772774	−0.0372472399

		Q_9	Q_{10}	Q_{11}	Q_{12}	Q_{13}	Q_{14}	Q_{15}	Q_{16}
$\tilde{\nu}^{\mathrm{HO}}$		955.687	969.635	1083.808	1099.884	1254.880	1257.923	1405.225	1407.720
	$l_{\alpha_i,j}$:								
c_{1x}	0.2868654398	0	0	0	0	0.0662994950	0.0769799509	0.1502666881	0.1765604364
c_{1y}	0	−0.0247296491	−0.0473246894	0.1775679438	0.1730731049	0	0	0	0
c_{1z}	−5.6564792624	0	0	0	0	−0.0249575215	−0.02444924822	0.0323523955	0.0266266895
c_{2x}	−2.1440160385	0	0	0	0	0.0687695806	0.07928842517	0.0766030777	0.0349121374
c_{2y}	0	0.2324148735	0.2089462462	0.0600001271	0.0997235577	0	0	0	0
c_{2z}	−0.8915699548	0	0	0	0	0.0146295325	0.01710606874	−0.0023710258	0.0054412768
c_{5x}	−2.1349725967	0	0	0	0	−0.0336695746	−0.03296837622	0.0047141652	0.0035566887
c_{5y}	0	−0.0161034747	−0.0173582869	0.0050915586	0.0020338197	0	0	0	0
c_{5z}	−2.7675548795	0	0	0	0	0.0137056925	0.01166829919	−0.0053390700	−0.0016912302
c_{6x}	2.1002784911	0	0	0	0	0.0109360953	0.00973205227	−0.0059207954	−0.0050318977
c_{6y}	0	−0.0024295085	−0.0128374699	0.0103028971	0.0062705186	0	0	0	0
c_{6z}	−2.2930907605	0	0	0	0	0.0090163634	0.00873518298	−0.0129775345	−0.0137694463
c_{9x}	0.2020375225	0	0	0	0	0.0212475911	0.01783137223	−0.0174254883	−0.0147863586
c_{9y}	0	0.0170175144	0.0266679760	−0.0386850254	−0.0339475088	0	0	0	0
c_{9z}	−3.5929593001	0	0	0	0	−0.0261151862	−0.02655809320	0.0218634733	0.014948154
c_{3x}	−0.2868649484	0	0	0	0	−0.0662239388	0.07701977435	0.1486994568	−0.177910191
c_{3y}	0	0.0248697099	−0.0472670316	−0.1776665890	0.1729598319	0	0	0	0
c_{3z}	5.6564793125	0	0	0	0	0.0249324436	−0.02447678207	0.0321180788	−0.026904760
c_{4x}	2.1440156985	0	0	0	0	−0.0686967410	0.07935782541	0.0763111573	−0.035554441
c_{4y}	0	−0.2330859635	0.2081969713	−0.0600960861	0.0996775320	0	0	0	0
c_{4z}	0.8915695806	0	0	0	0	−0.0146126018	0.01711941275	−0.0024192361	−0.005424255
c_{7x}	2.1349725840	0	0	0	0	0.0336369793	−0.03300183542	0.0046828284	−0.003595615
c_{7y}	0	0.0161600581	−0.0173094723	−0.0050906410	0.0020308739	0	0	0	0
c_{7z}	2.7675545069	0	0	0	0	−0.0136938047	0.01168167391	−0.0053256537	0.001732898
c_{8x}	−2.1002785866	0	0	0	0	−0.0109262153	0.00974346038	−0.0058748507	0.005085181
c_{8y}	0	0.0024723498	−0.0128328944	−0.0103056654	0.0062635652	0	0	0	0
c_{8z}	2.2930911271	0	0	0	0	−0.0090076076	0.00874641848	−0.0128548521	0.013883743
c_{10x}	−2.2020373912	0	0	0	0	−0.0212296035	0.01785354480	−0.0172972349	0.014933437
c_{10y}	0	−0.0171025155	0.0266218433	0.0387047148	−0.0339245550	0	0	0	0
c_{10z}	3.5929593354	0	0	0	0	0.0260887832	−0.02658517678	0.0217335486	−0.015133642

(Table I continued.)

		Q_{17}	Q_{18}	Q_{19}	Q_{20}	Q_{21}	Q_{22}	Q_{23}	Q_{24}
$\tilde{\nu}^{\mathrm{HO}}$		1447.463	1480.190	1713.868	1778.743	3094.003	3095.465	3231.252	3325.172
	$l_{\alpha_i,j}$:								
c_{1x}	0.2868654398	−0.1014904934	0.0539458530	−0.0271137400	0.0294157509	−0.0068577124	0.00690398212	−0.0036229233	−0.0006193951
c_{1y}	0	0	0	0	0	0	0	0	0
c_{1z}	−5.6564792624	0.0048179202	−0.0095596860	0.0230512400	−0.0176567618	0.1336263016	0.13096390621	0.0074510990	0.0132394726
c_{2x}	−2.1440160385	0.1520891779	−0.1613601303	0.0507020049	−0.0291244301	−0.0012160887	0.00024199369	−0.0056173447	−0.0058632848
c_{2y}	0	0	0	0	0	0	0	0	0
c_{2z}	−0.8915699548	−0.0071891429	0.0015851962	−0.0125699147	−0.0021036311	−0.0078113561	0.01374766678	0.1310048828	0.1290683147
c_{5x}	−2.1349725967	−0.0027699692	0.0017714739	−0.0059881835	0.0071063221	−0.0000570353	0.00007000256	−0.0004064703	0.0004206479
c_{5y}	0	0	0	0	0	0	0	0	0
c_{5z}	−2.7675548795	−0.0136379583	0.0134229069	−0.0009824420	0.0007835486	0.0005762451	−0.00101054142	−0.0083322496	−0.0082008171
c_{6x}	2.1002784911	0.0086457275	−0.0125342624	−0.0203379601	0.0207555405	0.0003841836	−0.00021343281	−0.0011630504	0.0001235220
c_{6y}	0	0	0	0	0	0	0	0	0
c_{6z}	−2.2930907605	0.0073392025	−0.0038895304	−0.0146475416	0.0144639245	0.0003754058	−0.00018770156	−0.0008181932	0.0001143304
c_{9x}	0.2020375225	−0.0120715877	0.0194227157	0.0345250080	−0.0371287112	0.0002009448	−0.00040886758	0.0025824167	−0.0001807620
c_{9y}	0	0	0	0	0	0	0	0	0
c_{9z}	−3.5929593001	0.0085878496	−0.0099552073	0.0225977040	−0.0186472428	−0.0117622828	0.01143198020	−0.0005022856	−0.0011721340
c_{3x}	−0.2868649484	−0.1014723075	−0.0539182353	0.0271121764	0.0294144790	0.0067396231	0.00701871764	0.0036224445	−0.0006193446
c_{3y}	0	0	0	0	0	0	0	0	0
c_{3z}	5.6564793125	0.0048307456	0.0095549130	−0.0230507487	−0.0176565925	−0.1313978519	−0.13319919832	−0.0074485992	0.0132389046
c_{4x}	2.1440156985	0.1521756753	0.1612764888	−0.0506980876	−0.0291213946	0.0012117706	0.00026242782	0.0056168386	−0.0058647308
c_{4y}	0	0	0	0	0	0	0	0	0
c_{4z}	0.8915695806	−0.0071893064	−0.0015809639	0.0125692787	−0.0021041803	0.0075769931	0.01387625596	−0.1309923064	0.1290810446
c_{7x}	2.1349725840	−0.0027695478	−0.0017703710	0.0059882525	0.0071061085	0.0000558376	0.00007096286	0.0004065357	0.0004206417
c_{7y}	0	0	0	0	0	0	0	0	0
c_{7z}	2.7675545069	−0.0136455848	−0.0134166519	0.0009823348	0.0007835908	−0.0005590306	−0.00102001048	0.0083313875	−0.0082015189
c_{8x}	−2.1002785866	0.0086495091	0.0125302330	0.0203386057	0.0207554315	−0.0003804949	−0.00021986770	0.0011630137	0.0001234232
c_{8y}	0	0	0	0	0	0	0	0	0
c_{8z}	2.2930911271	0.0073371909	0.0038873291	0.0146478186	0.0144637009	−0.0003721938	−0.00019400829	0.0008181618	0.0001142268
c_{10x}	−0.2020373912	−0.0120840852	−0.0194152472	−0.0345258830	−0.0371283550	−0.0001939268	−0.00041227494	−0.0025823641	−0.0001805188
c_{10y}	0	0	0	0	0	0	0	0	0
c_{10z}	3.5929593354	0.0085976123	0.0099501442	−0.0225979539	−0.0186468512	0.0115676507	0.01162842543	0.0005020965	−0.0011721186

(Table I continued.)

TABLE II. Curvilinear normal coordinate definition of FAD corresponding to the QB16-PES and the internal coordinate definition of Sec. II.A: equilibrium value of the internal coordinates $\xi_i^{(\mathrm{eq})}$ with $i = 1, \ldots, 6$ and $\mathcal{L}_{i,j}$ coefficients ($j = 1, \ldots, 6$) corresponding to the $\mathcal{Q}_j$ curvilinear normal coordinates. The harmonic frequencies, $\tilde{\nu}^{\mathrm{HO}}$ in cm^{-1}, are also given in the table. $\xi_i = \xi_i^{(\mathrm{eq})} + \sum_{j=1}^{6} \mathcal{Q}_j \mathcal{L}_{i,j}$

		$\mathcal{Q}_1$	$\mathcal{Q}_2$	$\mathcal{Q}_3$	$\mathcal{Q}_4$	$\mathcal{Q}_5$	$\mathcal{Q}_6$
$\tilde{\nu}^{\mathrm{HO}}$		65.757	155.438	160.447	222.384	262.267	328.281
	$\mathcal{L}_{i,j}$:						
R	5.6805167586	0	−0.0000000490	0	0.1480298121	0.0078114080	0
$\cos\theta$	−0.3330272401	0	−0.0344289689	0	0.0119751350	−0.0482796603	0
ϕ	4.7123889804	0.0890745125	0	0.0926450828	0	0	0.0616821979
α	3.1415926536	0.0101279780	0	−0.1158548265	0	0	0.0947600155
$\cos\beta$	0.3330274046	0	−0.0344289590	0	−0.0119753490	0.0482796630	0
γ	1.5707963268	−0.0931639847	0	0.0759836591	0	0	0.0692761166

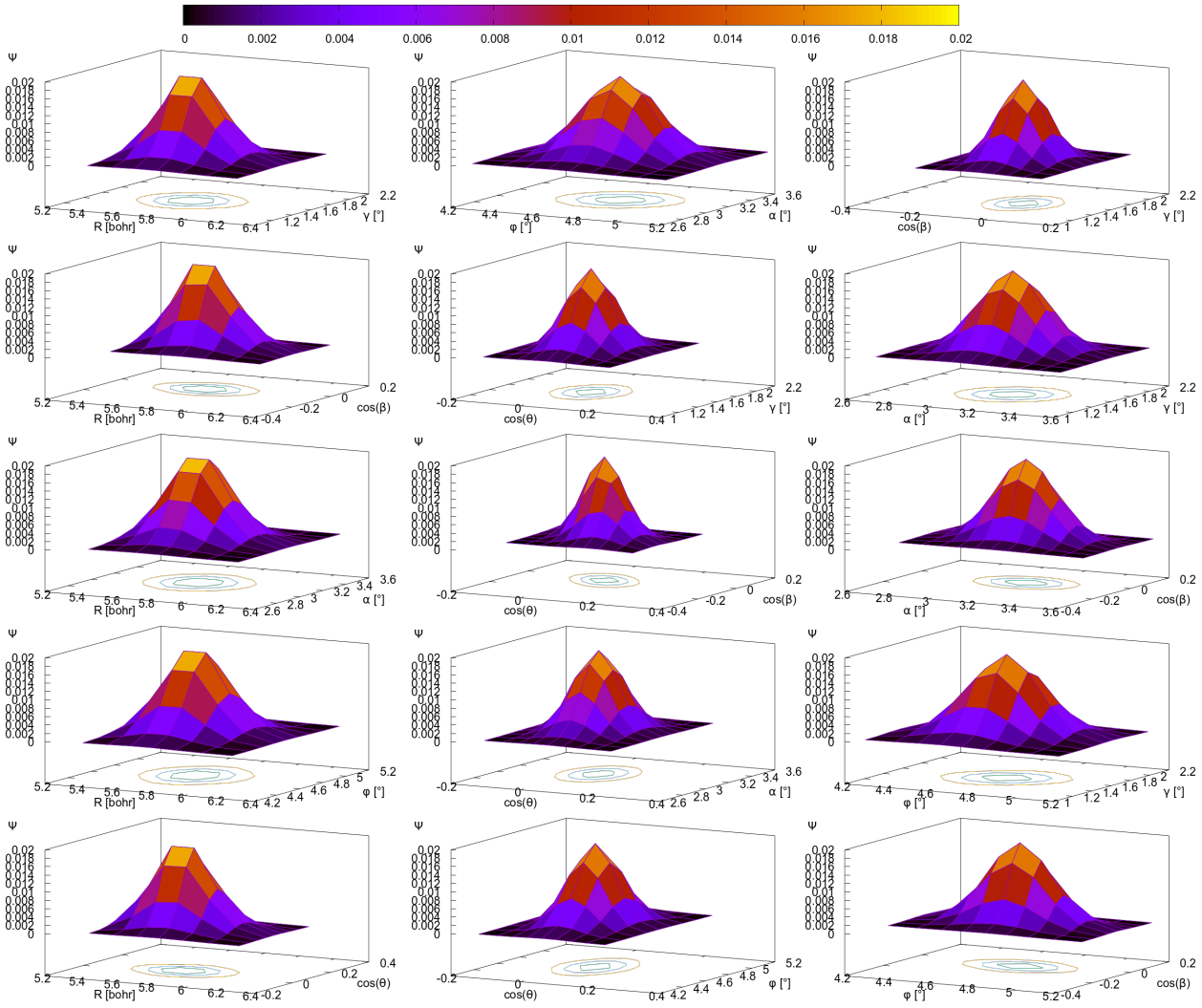

FIG. 1. Ψ_0 with $\tilde{\nu}_0 = 1532.9$ cm^{-1} obtained with GENIUSH using the 8D($\mathcal{I}$t) curvilinear KEO and the QB16-PES.

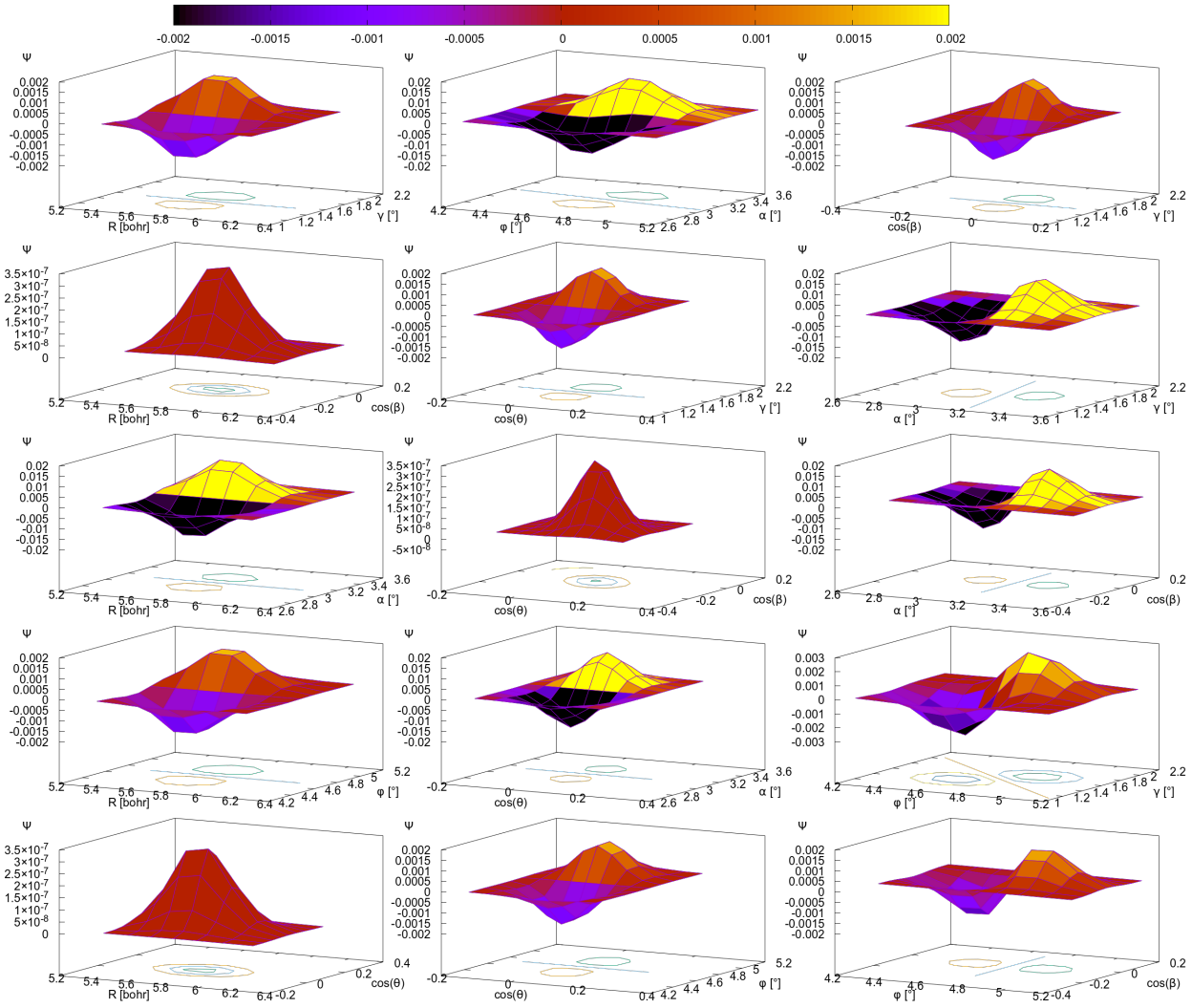

FIG. 2. Ψ_1 with $\tilde{\nu}_1 - \tilde{\nu}_0 = 70.5$ cm^{-1} (see also caption to Figure 1).

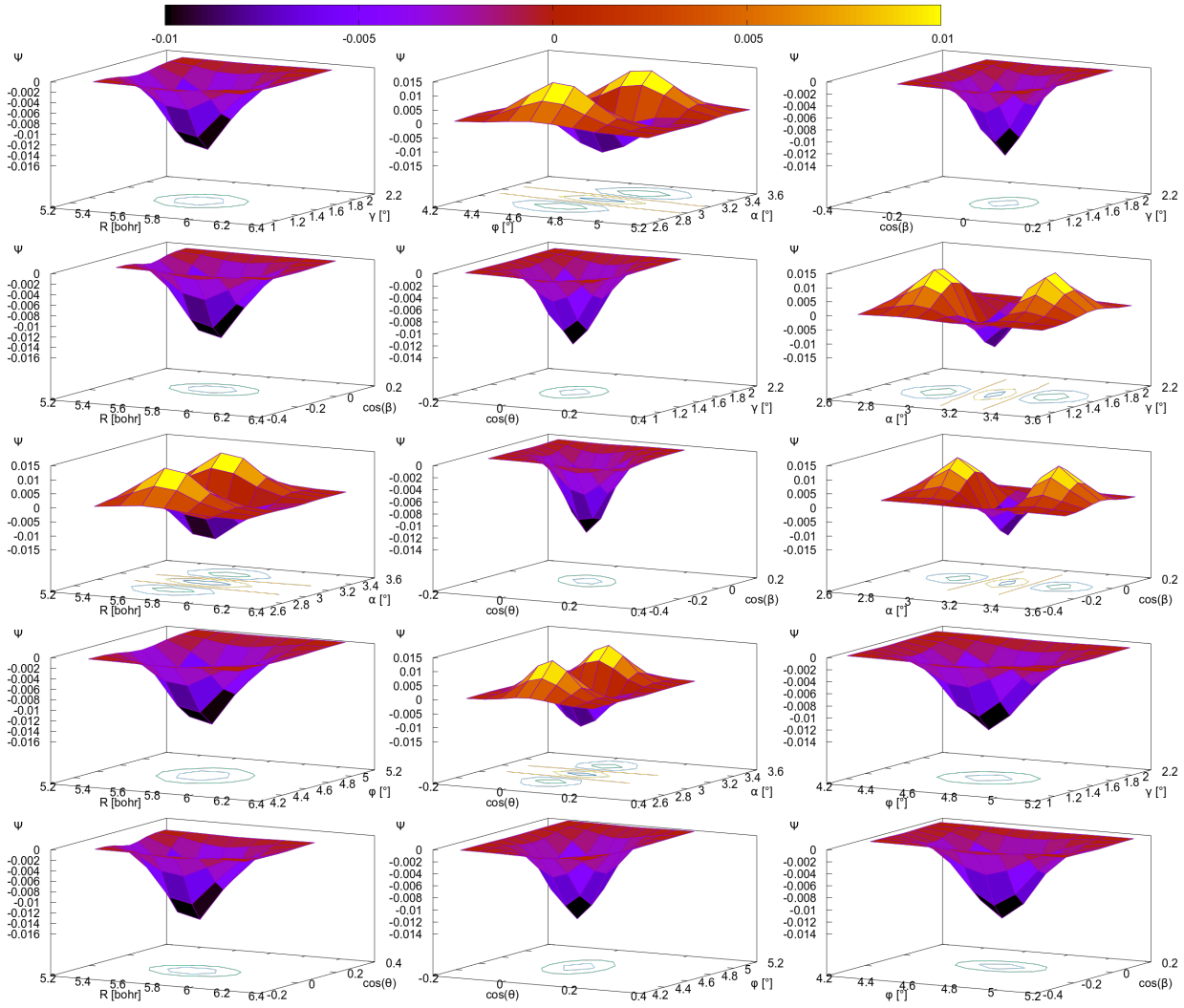

FIG. 3. Ψ_2 with $\tilde{\nu}_2 - \tilde{\nu}_0 = 140.9$ cm^{-1} (see also caption to Figure 1).

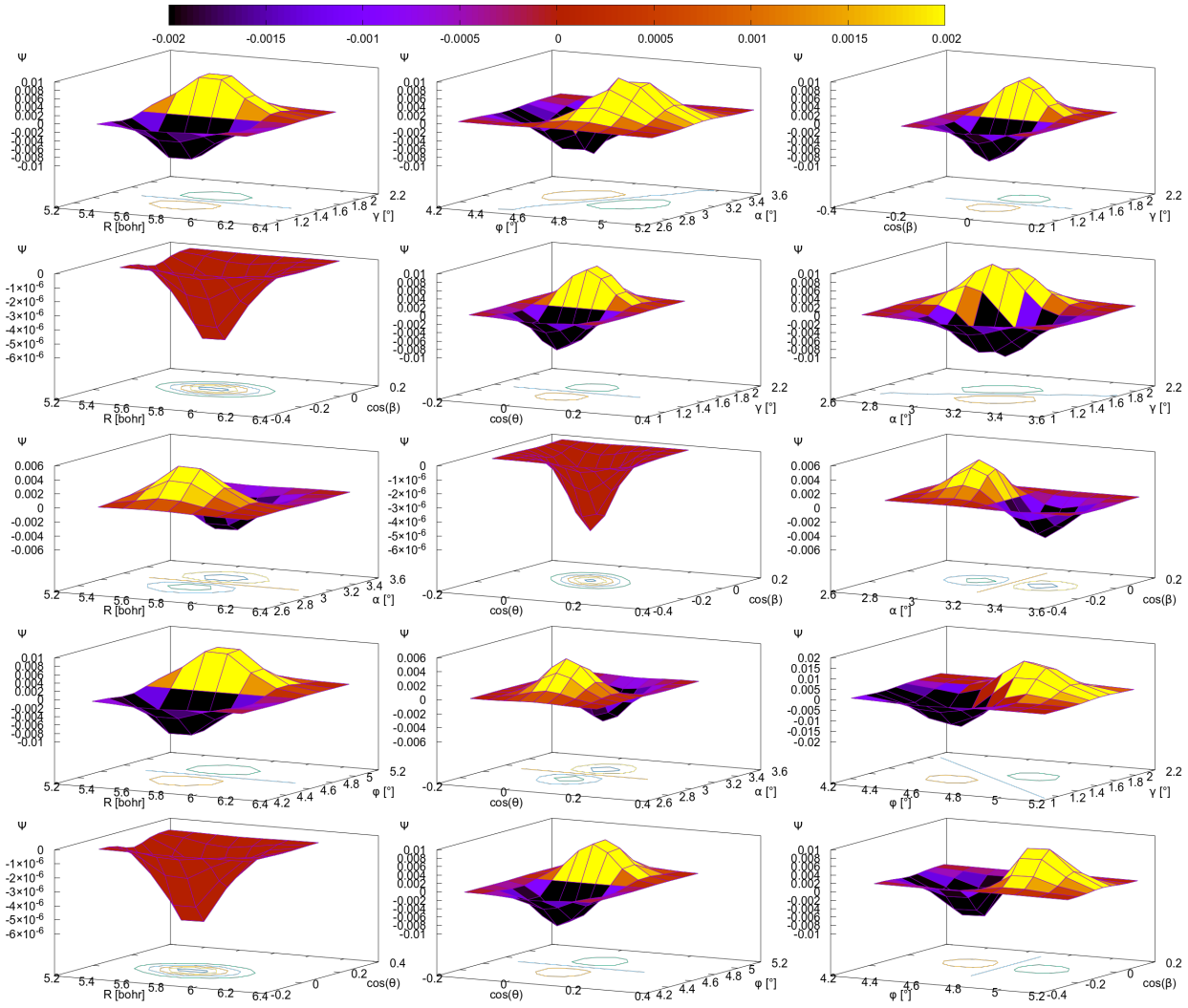

FIG. 4. Ψ_3 with $\tilde{\nu}_3 - \tilde{\nu}_0 = 162.2$ cm^{-1} (see also caption to Figure 1).

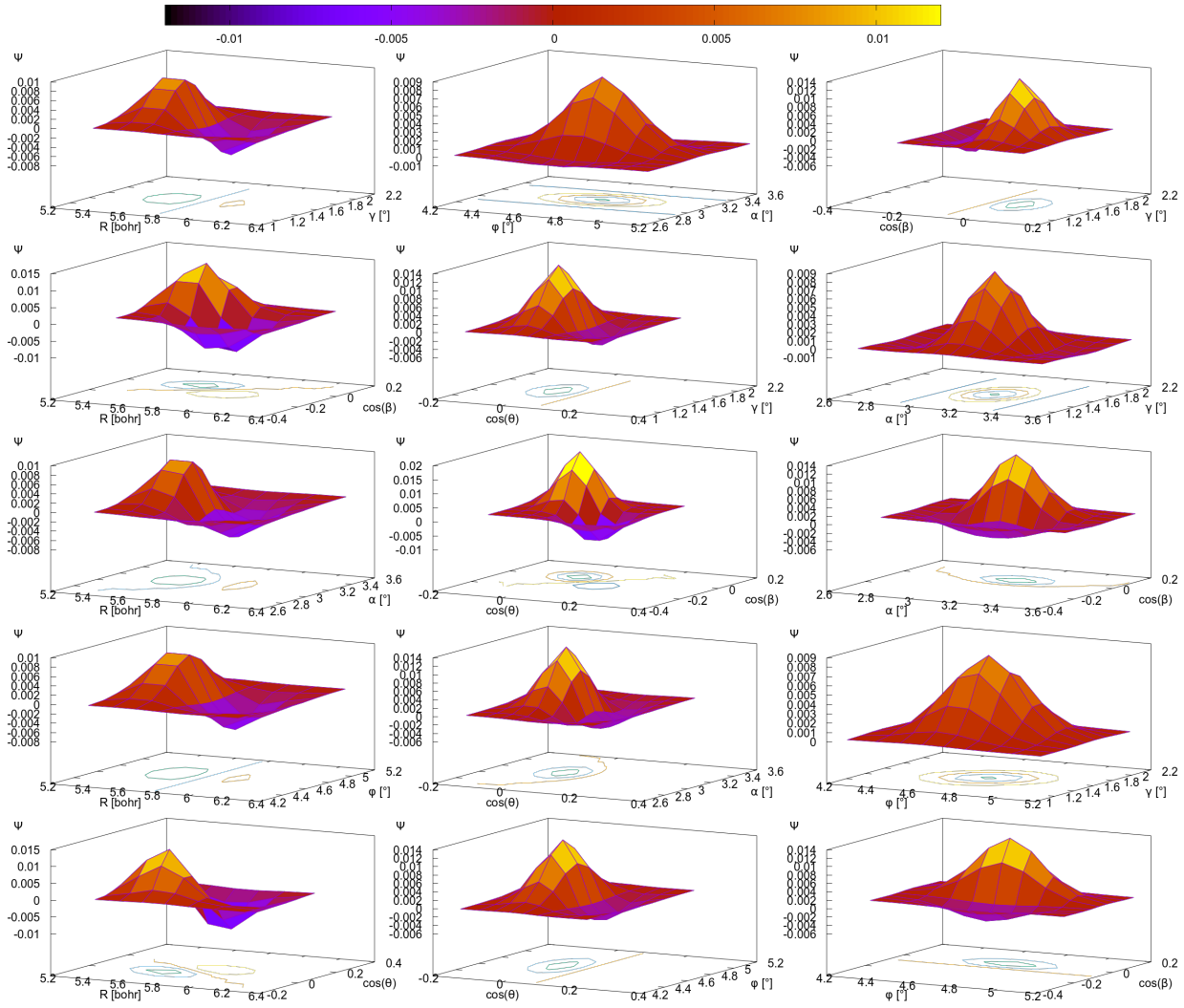

FIG. 5. Ψ_4 with $\tilde{\nu}_4 - \tilde{\nu}_0 = 191.4$ cm^{-1} (see also caption to Figure 1).

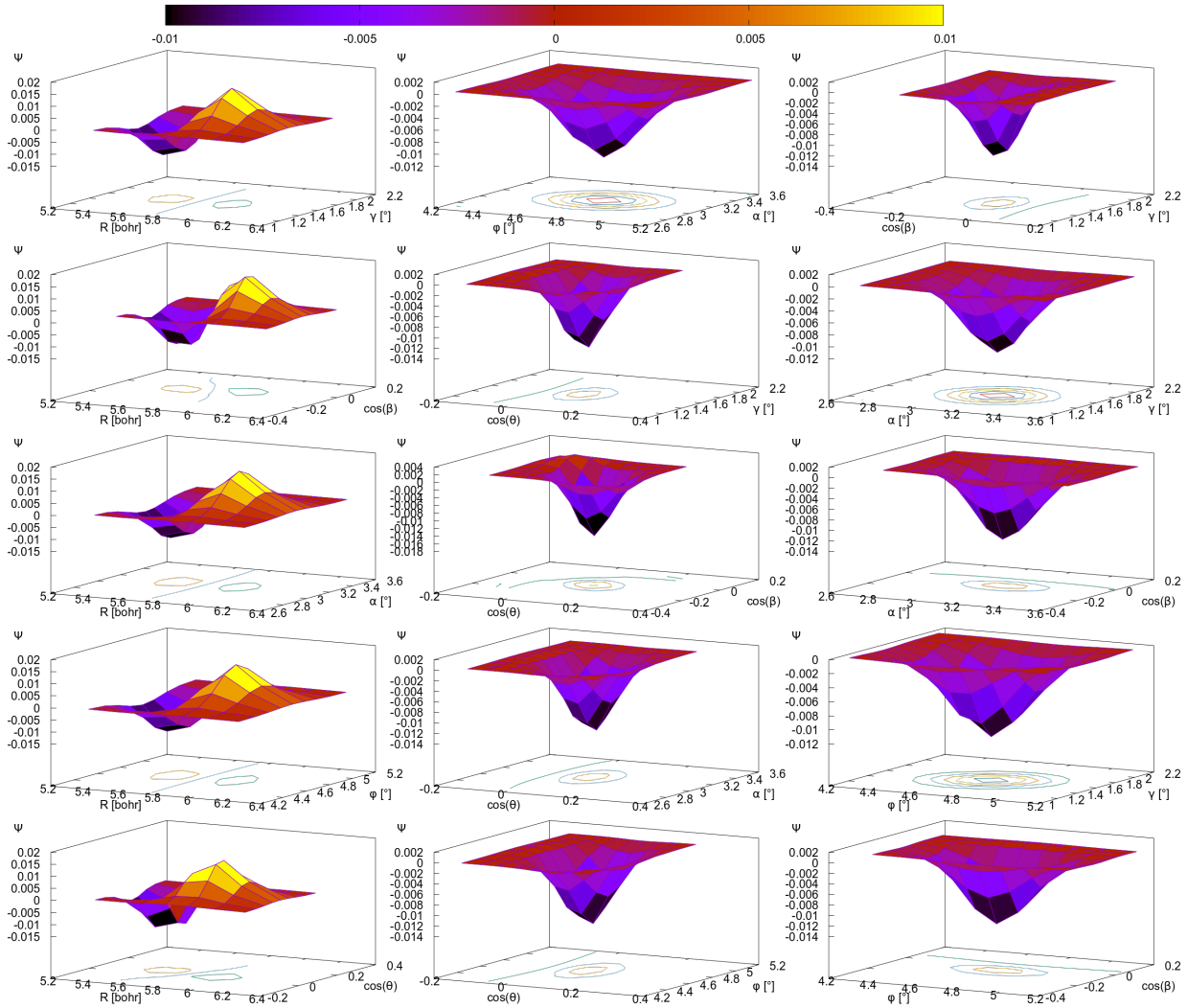

FIG. 6. Ψ_5 with $\tilde{\nu}_5 - \tilde{\nu}_0 = 207.7$ cm^{-1} (see also caption to Figure 1).

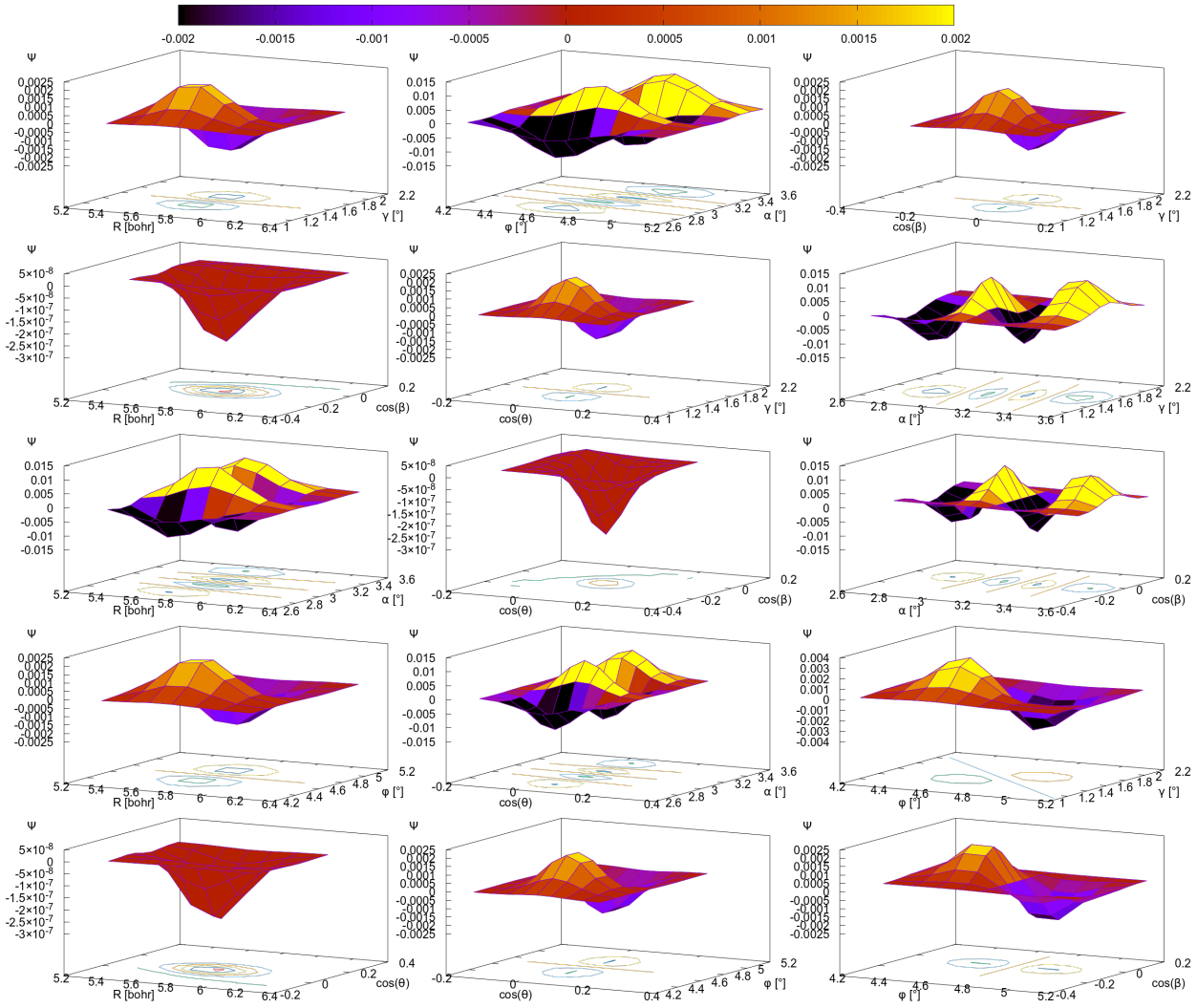

FIG. 7. Ψ_6 with $\tilde{\nu}_6 - \tilde{\nu}_0 = 211.1$ cm^{-1} (see also caption to Figure 1).

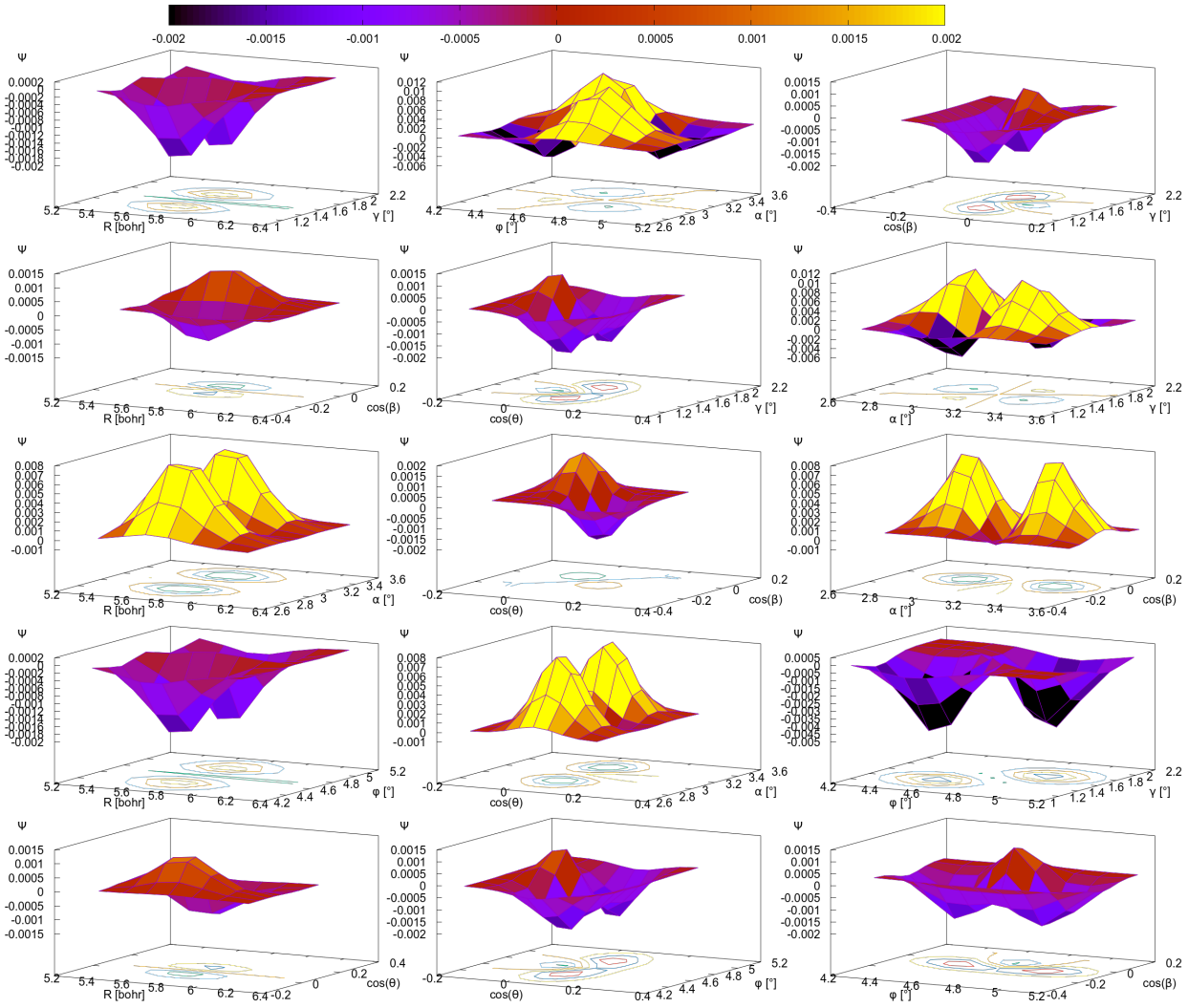

FIG. 8. Ψ_7 with $\tilde{\nu}_7 - \tilde{\nu}_0 = 232.6$ cm^{-1} (see also caption to Figure 1).

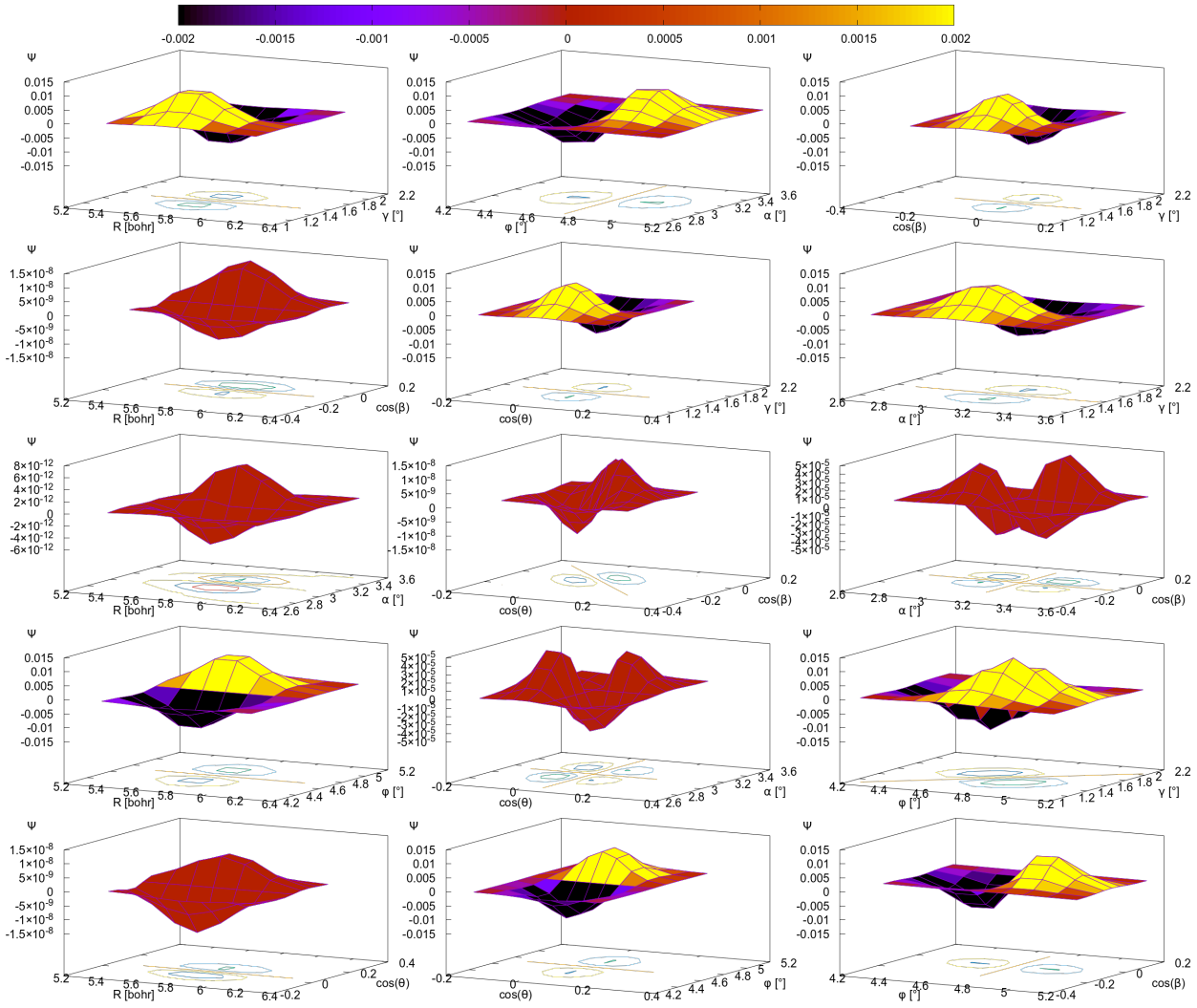

FIG. 9. Ψ_8 with $\tilde{\nu}_8 - \tilde{\nu}_0 = 239.4$ cm^{-1} (see also caption to Figure 1).

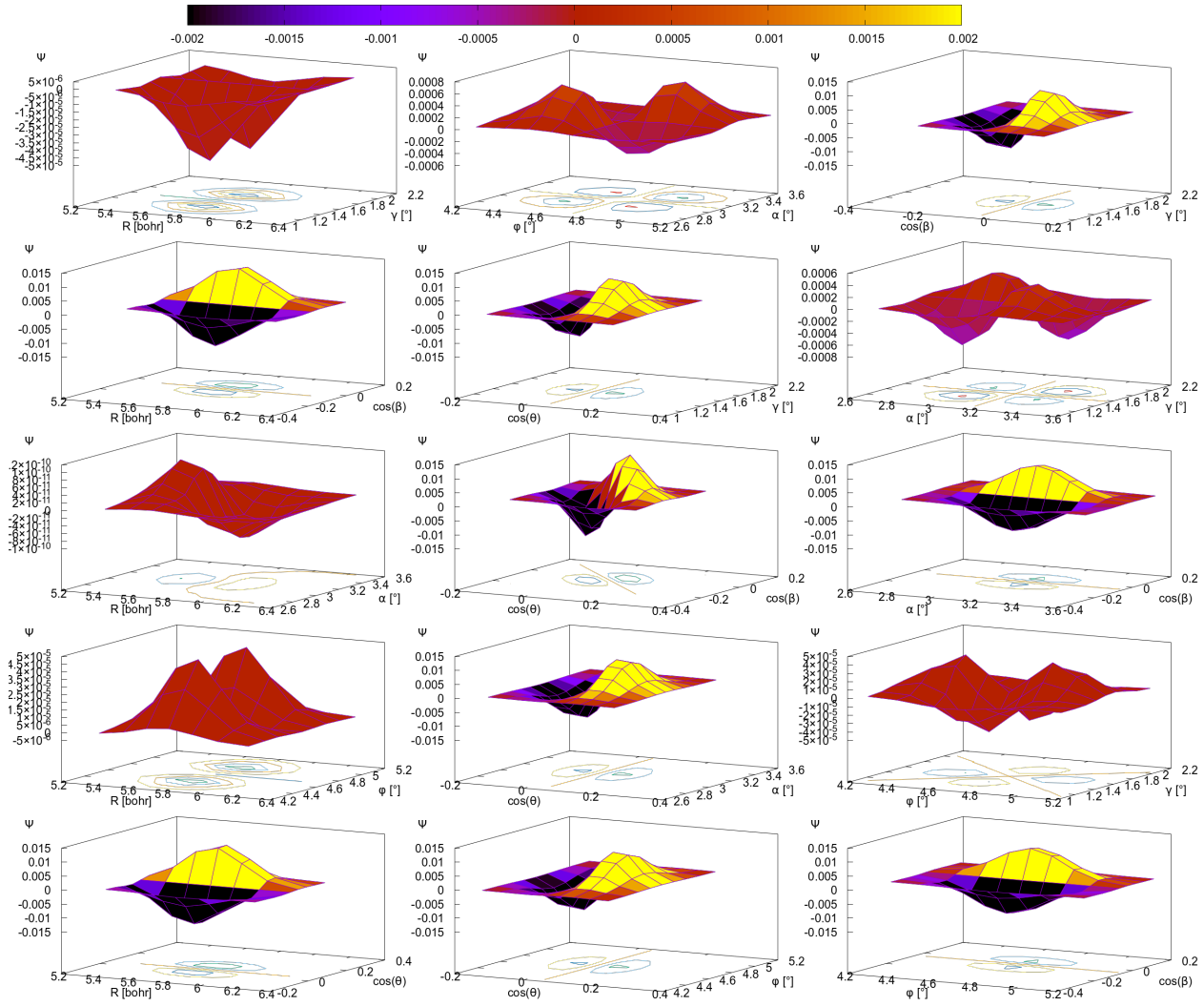

FIG. 10. Ψ_9 with $\tilde{\nu}_9 - \tilde{\nu}_0 = 253.5$ cm^{-1} (see also caption to Figure 1).

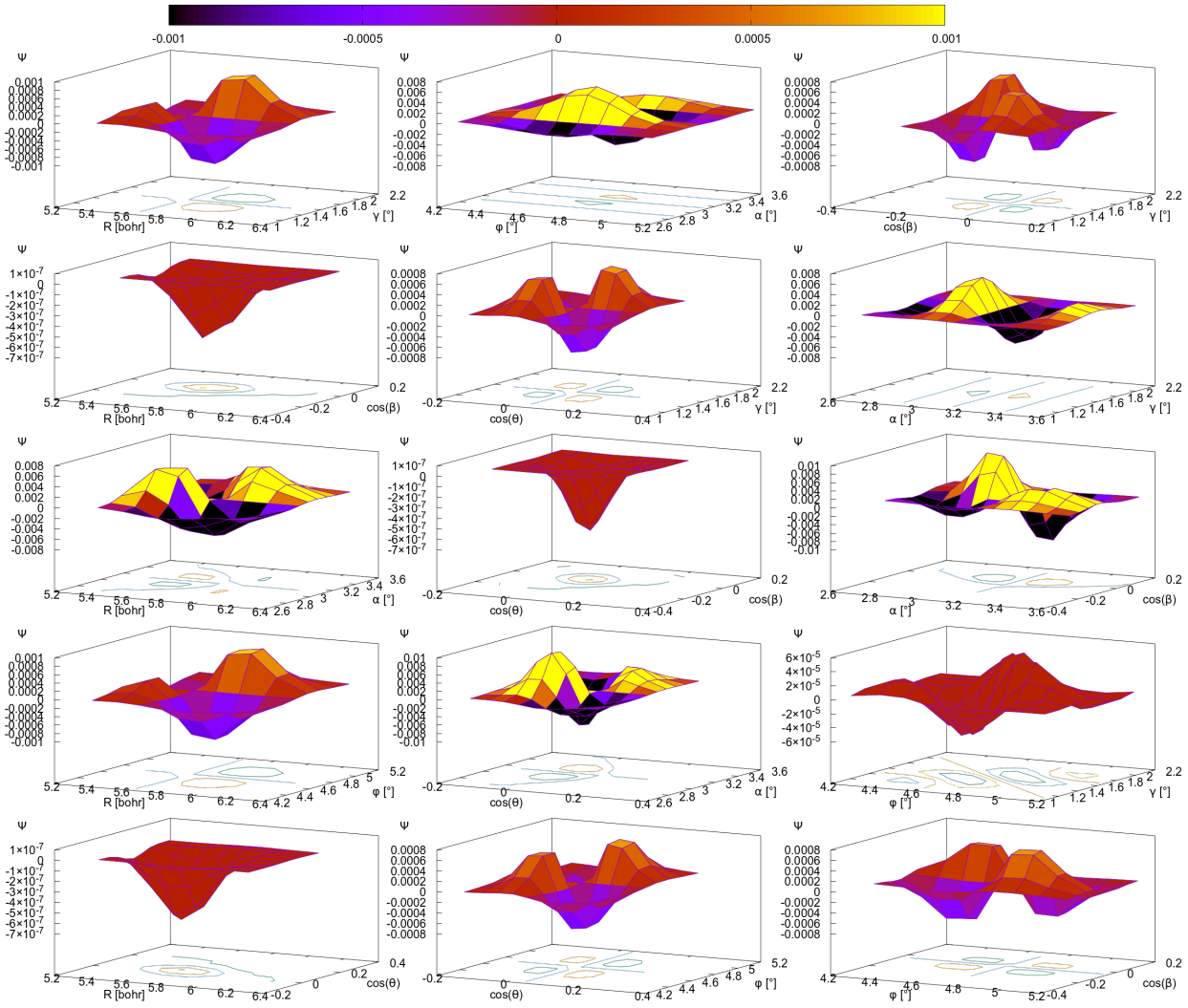

FIG. 11. Ψ_{10} with $\tilde{\nu}_{10} - \tilde{\nu}_0 = 262.0$ cm^{-1} (see also caption to Figure 1).

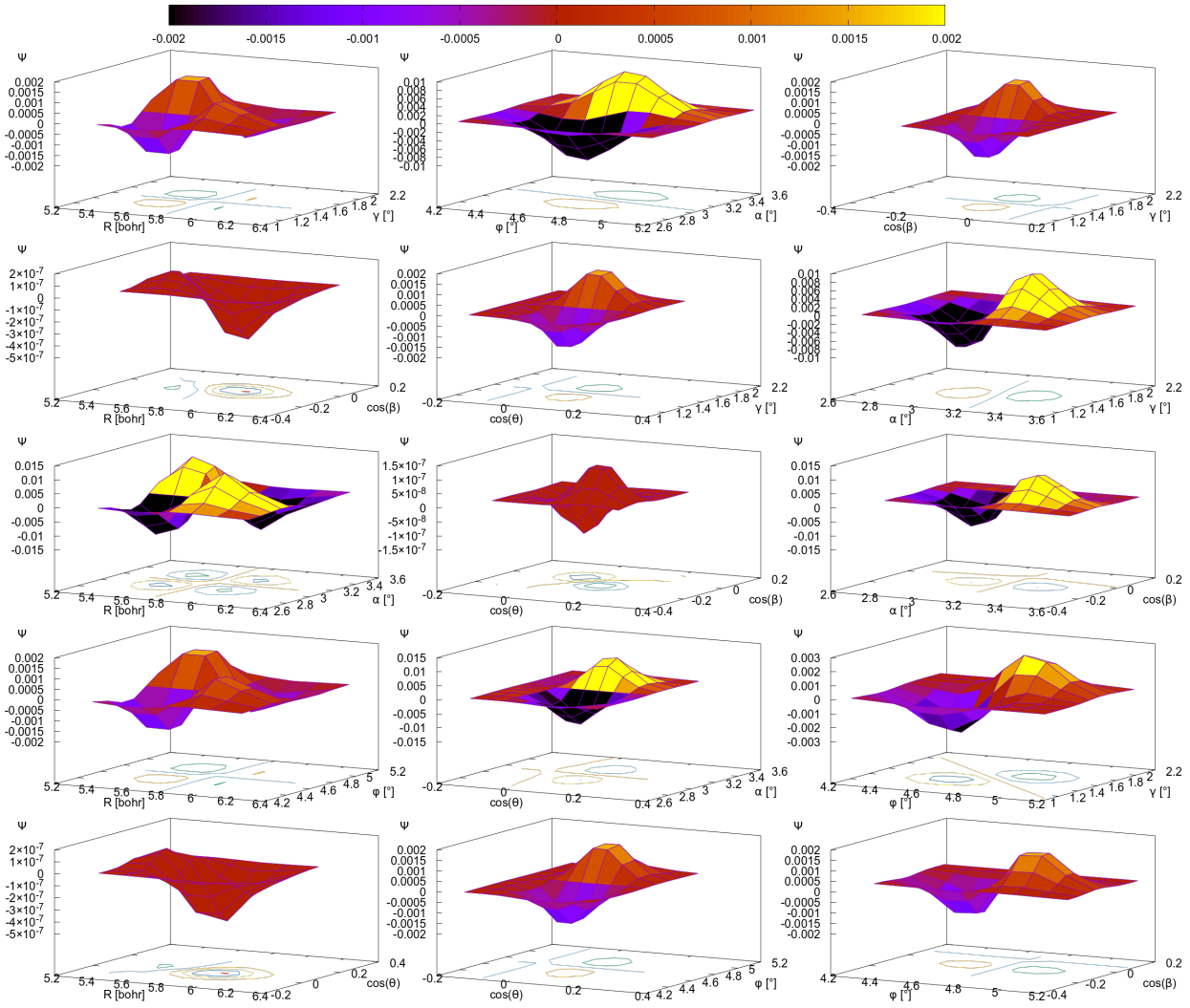

FIG. 12. Ψ_{11} with $\tilde{\nu}_{11} - \tilde{\nu}_0 = 277.3$ cm^{-1} (see also caption to Figure 1).

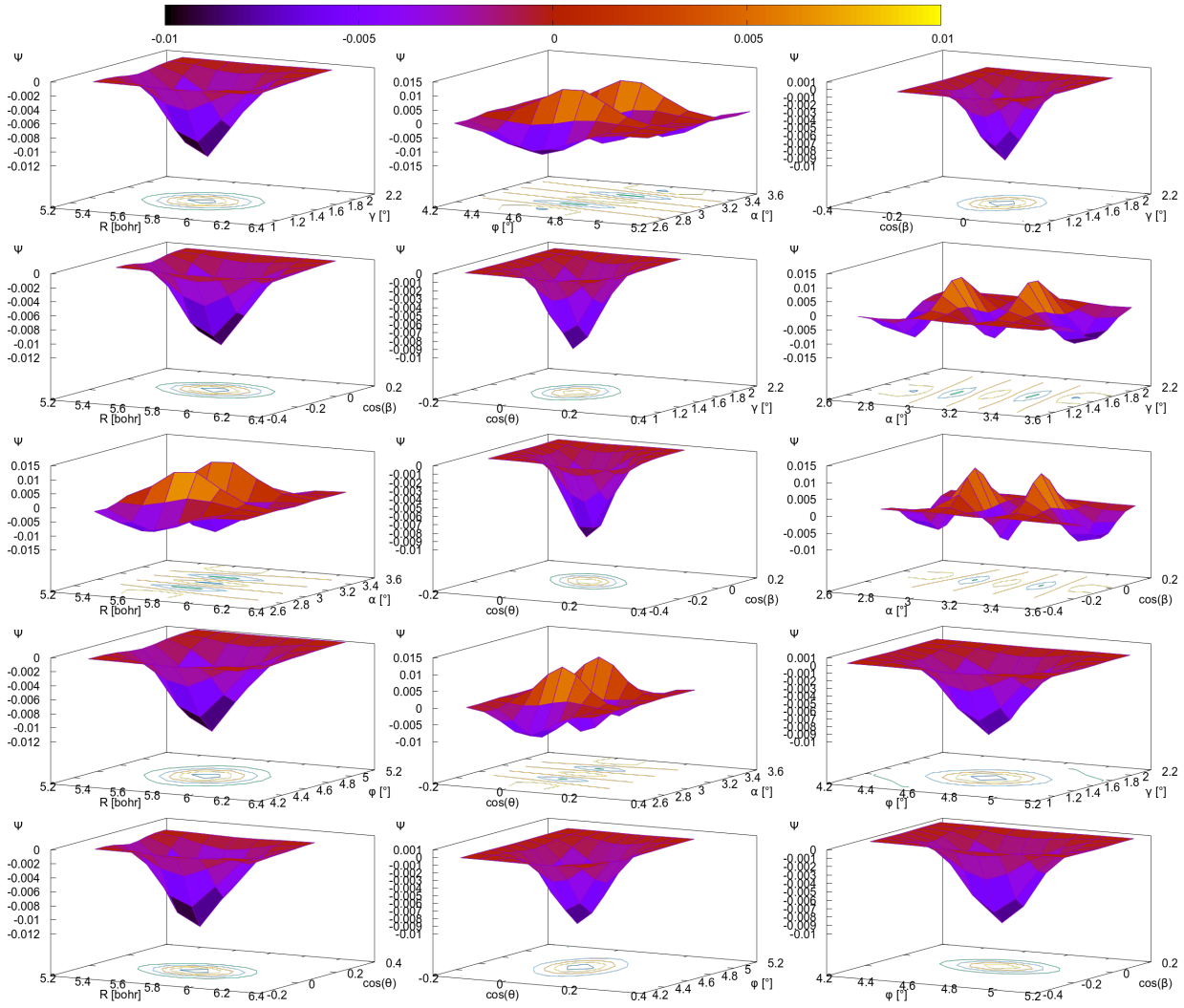

FIG. 13. Ψ_{12} with $\tilde{\nu}_{12} - \tilde{\nu}_0 = 280.4$ cm^{-1} (see also caption to Figure 1).

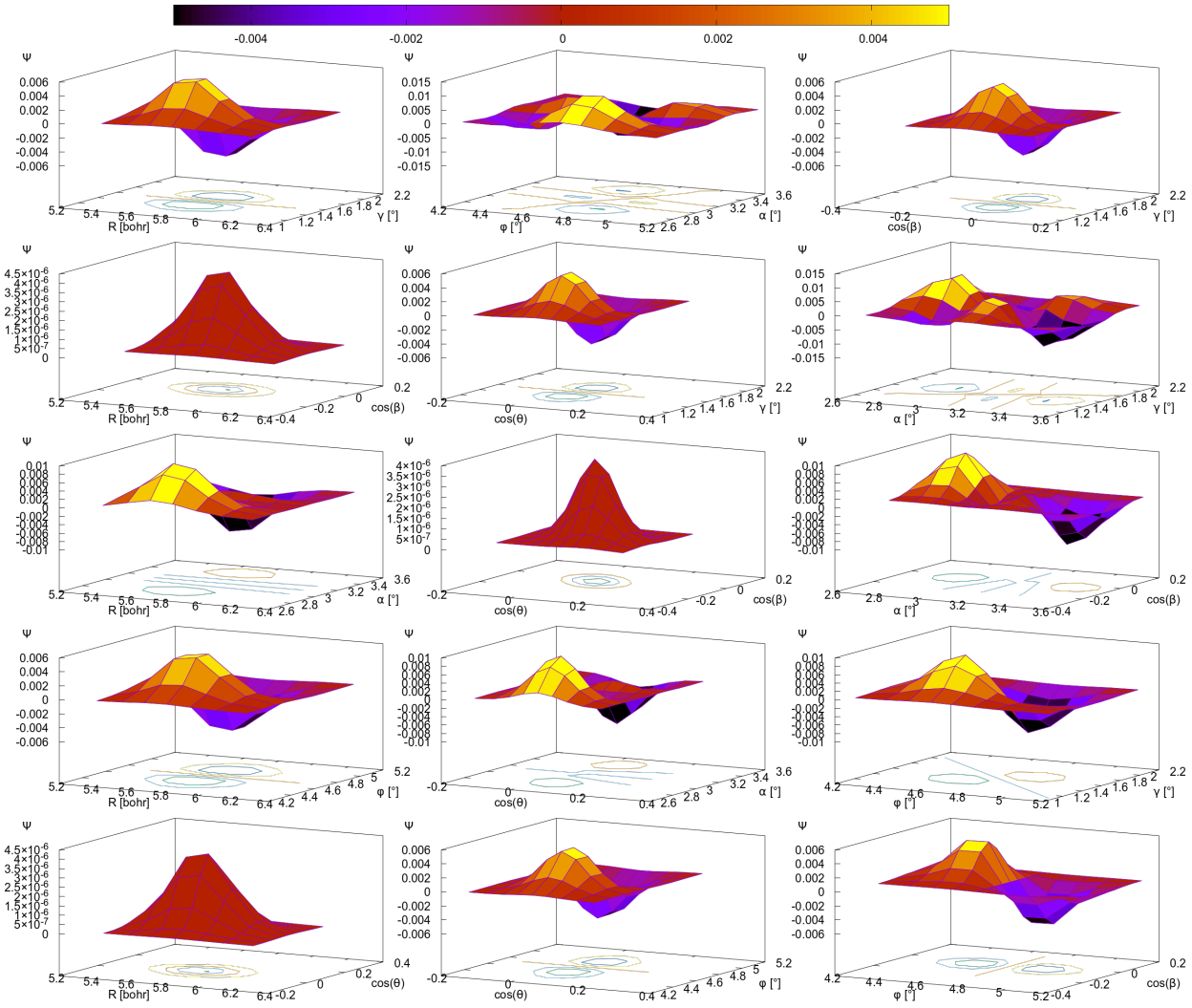

FIG. 14. Ψ_{13} with $\tilde{\nu}_{13} - \tilde{\nu}_0 = 302.9$ cm^{-1} (see also caption to Figure 1).

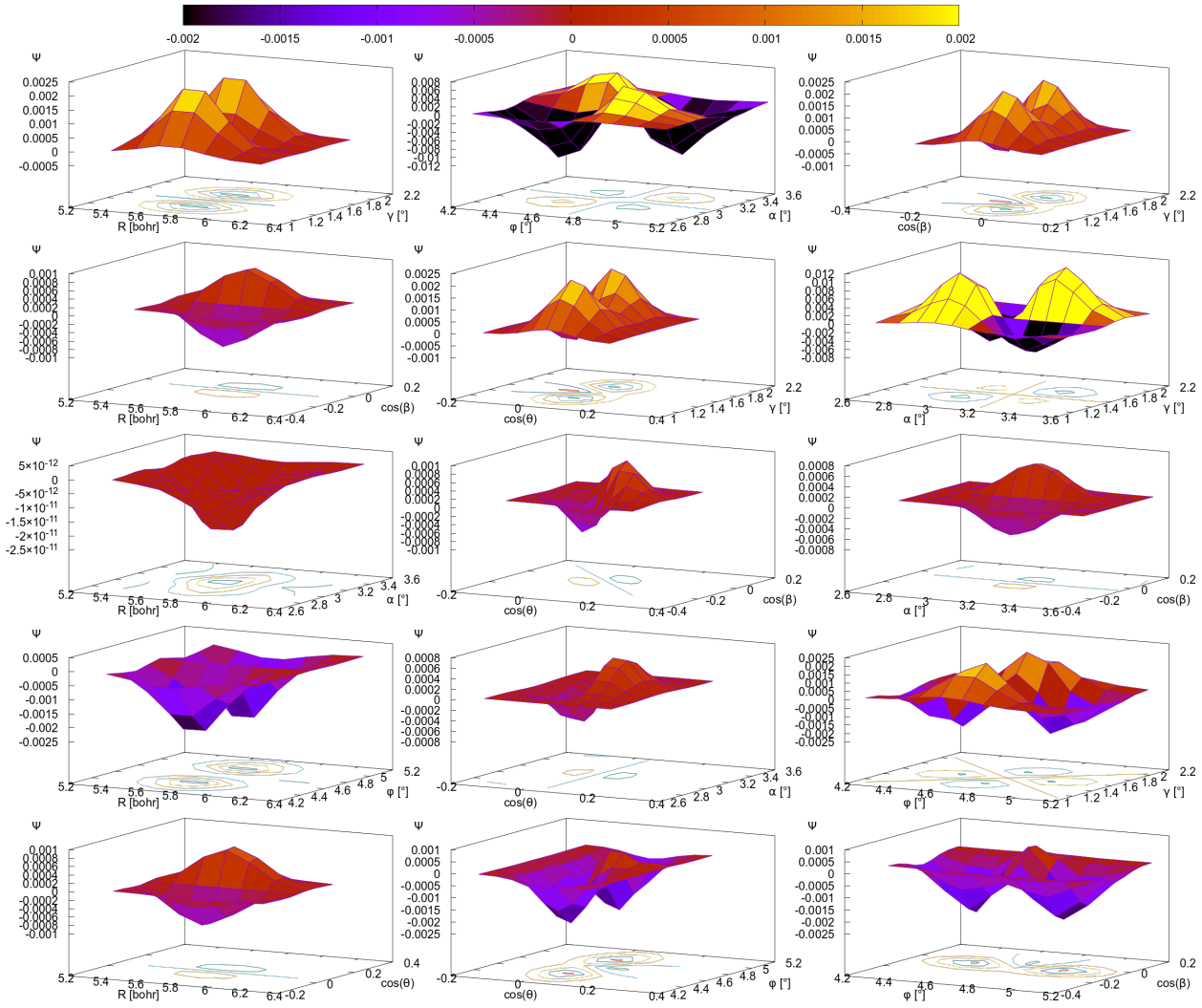

FIG. 15. Ψ_{14} with $\tilde{\nu}_{14} - \tilde{\nu}_0 = 309.8$ cm^{-1} (see also caption to Figure 1).