Supplementary Tables for Analytic Three-Dimensional 'MLR' Potential Energy Surface for CO_2-He, and Its Predicted Microwave and Infrared Spectra

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Table A-1. Comparison of pure rotation level spacings of $CO_2(v_3 = 0)$-He calculated from our vibrationally averaged 2D PES, with experimental values defined as differences between observed infrared transitionsc[a] with a common upper state.

levels		original 2D PES		R_e-morphed PES	
$J'_{K'_aK'_c} - J''_{K''_aK''_c}$	obs.	calc.	diff.	calc.	diff.
$1_{01} - 0_{00}$	0.5916	0.5881	−0.0035	0.5915	−0.0001
$2_{02} - 0_{00}$	1.5836	1.5782	−0.0054	1.5841	0.0005
$2_{20} - 0_{00}$	2.4497	2.4425	−0.0072	2.4506	0.0009
$2_{21} - 1_{01}$	1.6748	1.6755	0.0007	1.6760	0.0012
$3_{03} - 1_{01}$	2.3392	2.3323	−0.0069	2.3388	−0.0004
$2_{20} - 2_{02}$	0.8661	0.8644	−0.0017	0.8665	0.0004
$3_{22} - 2_{02}$	2.3997	2.3922	−0.0075	2.3995	−0.0002
$4_{04} - 2_{02}$	3.0667	3.0547	−0.0120	3.0642	−0.0025
$3_{22} - 2_{20}$	1.5345	1.5279	−0.0066	1.5330	−0.0015
$3_{03} - 2_{21}$	0.6653	0.6568	−0.0085	0.6628	−0.0025
$3_{21} - 2_{21}$	2.3020	2.2795	−0.0225	2.2983	−0.0037
$4_{41} - 2_{21}$	5.6243	5.6166	−0.0077	5.6230	−0.0013
$3_{21} - 3_{03}$	1.6367	1.6226	−0.0141	1.6356	−0.0011
$4_{23} - 3_{03}$	3.2037	3.1901	−0.0136	3.2022	−0.0015
$5_{05} - 3_{03}$	3.8131	3.7965	−0.0166	3.8088	−0.0043
$4_{23} - 3_{21}$	1.5665	1.5674	0.0009	1.5666	0.0001
$4_{41} - 3_{21}$	3.3223	3.3371	0.0148	3.3246	0.0023
$4_{04} - 3_{22}$	0.6664	0.6624	−0.0040	0.6647	−0.0017
$4_{22} - 3_{22}$	3.2192	3.1990	−0.0202	3.2171	−0.0021
$4_{22} - 4_{04}$	2.5538	2.5366	−0.0172	2.5524	−0.0014
$5_{24} - 4_{04}$	4.0051	3.9892	−0.0159	4.0041	−0.0010
$6_{06} - 4_{04}$	4.5560	4.5369	−0.0191	4.5517	−0.0043
$4_{40} - 4_{22}$	0.7777	0.7919	0.0142	0.7776	−0.0001
$5_{24} - 4_{22}$	1.4513	1.4526	0.0013	1.4517	0.0004
$4_{41} - 4_{23}$	1.7552	1.7697	0.0145	1.7580	0.0028
$5_{05} - 4_{23}$	0.6094	0.6065	−0.0029	0.6067	−0.0027
$5_{23} - 4_{23}$	3.9142	3.9002	−0.0140	3.9094	−0.0048
$6_{25} - 4_{23}$	5.3912	5.3698	−0.0214	5.3868	−0.0044
$6_{25} - 5_{23}$	1.4770	1.4696	−0.0074	1.4775	0.0005
average			−0.0072		−0.0011
RMSD			0.0123		0.0022

[a] M. J. Weida, J. M. Sperhac, D. J. Nesbitt, and J. M. Hutson, J. Chem. Phys. **101**, 8351 (1994).

Table A-2. Comparison of pure rotation level spacings of $CO_2(v_3 = 1)$-He calculated from our vibrationally averaged 2D PES, with experimental values defined as differences between observed infrared transitions[a] with a common lower state.

levels		original 2D PES		R_e-morphed PES	
$J'_{K'_a K'_c} - J''_{K''_a K''_c}$	obs.	calc.	diff.	calc.	diff.
$2_{12} - 1_{10}$	0.7390	0.7375	−0.0015	0.7396	0.0006.
$2_{11} - 1_{11}$	1.5896	1.5814	−0.0082	1.5923	0.0027.
$3_{13} - 2_{11}$	0.7106	0.7112	0.0006	0.7094	−0.0012.
$3_{31} - 2_{11}$	2.4694	2.4734	0.0040	2.4691	−0.0003.
$3_{30} - 2_{12}$	3.2577	3.2515	−0.0062	3.2604	0.0027.
$3_{12} - 2_{12}$	2.4511	2.4436	−0.0075	2.4545	0.0034.
$3_{30} - 3_{12}$	0.8066	0.8079	0.0013	0.8059	−0.0007.
$4_{14} - 3_{12}$	0.6140	0.6131	−0.0009	0.6127	−0.0013.
$4_{32} - 3_{12}$	3.0229	3.0167	−0.0062	3.0216	−0.0013.
$3_{31} - 3_{13}$	1.7591	1.7623	0.0032	1.7597	0.0006.
$4_{13} - 3_{13}$	3.2205	3.2124	−0.0081	3.2233	0.0028.
$4_{32} - 3_{30}$	2.2163	2.2088	−0.0075	2.2156	−0.0007.
$4_{13} - 3_{31}$	1.4611	1.4502	−0.0109	1.4636	0.0025.
$4_{31} - 3_{31}$	2.9320	2.9064	−0.0256	2.9353	0.0033.
$4_{31} - 4_{13}$	1.4711	1.4562	−0.0149	1.4717	0.0006.
$5_{15} - 4_{13}$	0.5825	0.5801	−0.0024	0.5815	−0.0010.
$5_{33} - 4_{13}$	3.7349	3.7175	−0.0174	3.7297	−0.0052.
$4_{32} - 4_{14}$	2.4087	2.4036	−0.0051	2.4089	0.0002.
$5_{14} - 4_{14}$	3.9742	3.9633	−0.0109	3.9765	0.0023.
$5_{33} - 4_{31}$	2.2643	2.2613	−0.0030	2.2580	−0.0063.
$5_{14} - 4_{32}$	1.5650	1.5597	−0.0053	1.5676	0.0026.
$6_{16} - 5_{14}$	0.5552	0.5526	−0.0026	0.5536	−0.0016.
average			−0.0061		0.0002
RMSD			0.0092		0.0025

[a] M. J. Weida, J. M. Sperhac, D. J. Nesbitt, and J. M. Hutson, J. Chem. Phys. **101**, 8351 (1994).

Table A-3. Comparison of calculated infrared transition frequencies for $^{12}C^{16}O_2$-He (in cm^{-1}) with experiment.[a]

potential :		original	morph R_e	morph R_e & $\mathfrak{D}_e$
$J'_{K'_a K'_c} - J''_{K''_a K''_c}$	observed	{calc. − obs.}	{calc. − obs.}	{calc. − obs.}
$6_{16} - 7_{07}$	2346.3788	−0.0177	−0.0269	0.0158
$5_{15} - 6_{06}$	2346.7611	−0.0302	−0.0385	0.0048
$4_{14} - 5_{05}$	2347.1394	−0.0342	−0.0411	0.0026
$3_{13} - 4_{04}$	2347.5141	−0.0388	−0.0446	−0.0007
$2_{12} - 3_{03}$	2347.8872	−0.0422	−0.0472	−0.0030
$1_{11} - 2_{02}$	2348.2810	−0.0436	−0.0490	−0.0045
$1_{10} - 1_{01}$	2349.4874	−0.0475	−0.0482	−0.0038
$2_{11} - 2_{02}$	2349.8702	−0.0514	−0.0459	−0.0018
$3_{12} - 3_{03}$	2350.3383	−0.0497	−0.0031	0.0002
$4_{13} - 4_{04}$	2350.7346	−0.0469	−0.0418	0.0019
$5_{14} - 5_{05}$	2351.1134	−0.0449	−0.0386	0.0046
$1_{11} - 0_{00}$	2349.8646	−0.0490	−0.0485	−0.0040
$2_{12} - 1_{01}$	2350.2264	−0.0491	−0.0476	−0.0034
$3_{13} - 2_{02}$	2350.5808	−0.0509	−0.0471	−0.0032
$4_{14} - 3_{03}$	2350.9525	−0.0508	−0.0454	−0.0017
$5_{15} - 4_{04}$	2351.3171	−0.0493	−0.0428	0.0005
$6_{16} - 5_{05}$	2351.6686	−0.0474	−0.0402	0.0025
$5_{14} - 6_{25}$	2346.3318	−0.0266	−0.0372	0.0060
$4_{13} - 5_{24}$	2346.7295	−0.0310	−0.0409	0.0029
$3_{12} - 4_{23}$	2347.1348	−0.0362	−0.0018	0.0015
$2_{11} - 3_{22}$	2347.4700	−0.0435	−0.0452	−0.0011
$1_{11} - 2_{20}$	2347.4149	−0.0419	−0.0495	−0.0050
$1_{10} - 2_{21}$	2347.8126	−0.0482	−0.0494	−0.0050
$2_{11} - 2_{20}$	2349.0045	−0.0501	−0.0468	−0.0027
$2_{12} - 2_{21}$	2348.5525	−0.0506	−0.0497	−0.0055
$3_{12} - 3_{21}$	2348.7015	−0.0355	−0.0019	0.0014
$3_{13} - 3_{22}$	2348.1808	−0.0431	−0.0466	−0.0027
$4_{13} - 4_{22}$	2348.1808	−0.0297	−0.0404	0.0033
$4_{14} - 4_{23}$	2347.7488	−0.0371	−0.0439	−0.0002
$5_{14} - 5_{23}$	2347.8088	−0.0340	−0.0367	0.0064
$3_{12} - 2_{21}$	2351.0036	−0.0581	−0.0056	−0.0023
$4_{13} - 3_{22}$	2351.4010	−0.0509	−0.0435	0.0002
$5_{14} - 4_{23}$	2351.7230	−0.0480	−0.0415	0.0016
$3_{31} - 4_{22}$	2346.7207	−0.0197	−0.0440	0.0005
$3_{30} - 3_{21}$	2349.5082	−0.0343	−0.0434	0.0006
$3_{31} - 3_{22}$	2349.9399	−0.0399	−0.0461	−0.0016
$4_{31} - 4_{22}$	2349.6519	−0.0446	−0.0399	0.0026
$4_{32} - 4_{23}$	2350.1580	−0.0427	−0.0442	−0.0011
$5_{33} - 5_{24}$	2350.4644	−0.0484	−0.0461	−0.0045
$3_{31} - 2_{20}$	2351.4744	−0.0466	−0.0476	−0.0032
$3_{30} - 2_{21}$	2351.8102	−0.0569	−0.0471	−0.0030
$4_{32} - 3_{21}$	2351.7245	−0.0418	−0.0441	−0.0010
$5_{33} - 4_{22}$	2351.9162	−0.0476	−0.0461	−0.0046
$3_{31} - 4_{40}$	2345.9430	−0.0340	−0.0439	0.0006
$3_{30} - 4_{41}$	2346.1859	−0.0491	−0.0457	−0.0017
$4_{31} - 4_{40}$	2348.8750	−0.0596	−0.0406	0.0019
$4_{32} - 4_{41}$	2348.4028	−0.0572	−0.0470	−0.0039
$3_{31} - 2_{02}$	2352.3396	−0.0474	−0.0463	−0.0018
$4_{32} - 3_{03}$	2353.3612	−0.0559	−0.0452	−0.0021
average	—	−0.0435	−0.0407	−0.0003
RMSD	—	0.0445	0.0424	0.0038

[a] M. J. Weida, J. M. Sperhac, D. J. Nesbitt, and J. M. Hutson, J. Chem. Phys. **101**, 8351 (1994).

Table A-4. Comparison with experiment[a] of infrared transition frequencies for $^{13}C^{16}O_2$-He and $^{12}C^{18}O_2$-He (in cm^{-1}) calculated using our final, fully morphed (w.r.t. R_e and $\mathfrak{D}_e$) potential.

$^{13}C^{16}O_2 - He$			$^{13}C^{18}O_2 - He$		
$J'_{K'_aK'_c} - J''_{K''_aK''_c}$	calc.	calc. − Obs.	$J'_{K'_aK'_c} - J''_{K''_aK''_c}$	calc.	calc. − Obs.
$1_{11} - 0_{00}$	2284.2024	−0.0013	$1_{01} - 0_{00}$	2247.9476	−0.0026
$1_{10} - 1_{01}$	2283.8257	−0.0005	$1_{10} - 1_{11}$	2247.5925	−0.0023
$2_{12} - 1_{01}$	2284.5647	−0.0009	$2_{12} - 1_{11}$	2248.2904	−0.0022
$1_{11} - 2_{02}$	2282.6197	−0.0019	$1_{01} - 2_{02}$	2246.4618	−0.0029
$2_{11} - 2_{02}$	2284.2090	0.0015	$2_{21} - 2_{02}$	2248.0461	−0.0001
$3_{13} - 2_{02}$	2284.9190	−0.0006	$3_{03} - 2_{02}$	2248.6516	−0.0017
$1_{10} - 2_{21}$	2282.1498	−0.0025	$3_{21} - 2_{02}$	2250.1654	−0.0011
$2_{12} - 2_{21}$	2282.8888	−0.0027	$1_{10} - 2_{11}$	2246.1119	−0.0034
$3_{12} - 2_{21}$	2285.3408	0.0004	$2_{12} - 2_{11}$	2246.8097	−0.0036
$3_{30} - 2_{21}$	2286.1475	0.0001	$3_{12} - 2_{11}$	2249.1020	−0.0012
$1_{11} - 2_{20}$	2281.7537	−0.0034	$3_{30} - 2_{11}$	2249.8802	−0.0006
$2_{11} - 2_{20}$	2283.3430	0.0000	$1_{01} - 2_{20}$	2245.6472	−0.0036
$3_{31} - 2_{20}$	2285.8145	0.0000	$2_{21} - 2_{20}$	2247.2315	−0.0007
$2_{12} - 3_{03}$	2282.2274	−0.0007	$3_{21} - 2_{20}$	2249.3508	−0.0015
$3_{12} - 3_{03}$	2284.6795	0.0020	$2_{12} - 3_{13}$	2246.1182	−0.0010
$4_{14} - 3_{03}$	2285.2921	0.0007	$3_{12} - 3_{13}$	2248.4105	0.0010
$2_{11} - 3_{22}$	2281.8112	0.0002	$4_{14} - 3_{13}$	2249.0028	0.0002
$3_{13} - 3_{22}$	2282.5212	−0.0007	$2_{21} - 3_{22}$	2245.7894	−0.0001
$3_{31} - 3_{22}$	2284.2827	0.0013	$3_{03} - 3_{22}$	2246.3949	−0.0010
$4_{13} - 3_{22}$	2285.7423	0.0029	$3_{21} - 3_{22}$	2247.9087	−0.0004
$3_{12} - 3_{21}$	2283.0471	0.0042	$4_{23} - 3_{22}$	2249.4020	0.0010
$3_{30} - 3_{21}$	2283.8538	0.0036	$3_{12} - 3_{31}$	2246.7335	0.0022
$3_{13} - 4_{04}$	2281.8570	0.0018	$3_{30} - 3_{31}$	2247.5117	0.0024
$5_{15} - 4_{04}$	2285.6589	0.0027	$3_{03} - 4_{04}$	2245.7668	0.0003
			$3_{21} - 4_{04}$	2247.2807	−0.0013
			$4_{23} - 4_{04}$	2248.7740	0.0024
			$5_{05} - 4_{04}$	2249.3415	−0.0108
			$3_{12} - 4_{13}$	2245.3845	0.0010
			$4_{14} - 4_{13}$	2245.9768	−0.0006
average{calc. − obs, }	—	0.0003		—	−0.0011
RMSD{calc. − obs, }	—	0.0020		—	0.0027

[a] M. J. Weida, J. M. Sperhac, D. J. Nesbitt, and J. M. Hutson, J. Chem. Phys. **101**, 8351 (1994).

Table A-5. Expansion coefficients $\overline{\mathfrak{D}}_e^{\lambda}$ [cm^{-1}], $\overline{R}_e^{\lambda}$ [Å] and $\overline{\beta}_i^{\lambda}$ defining our unmorphed two-dimensional vibrationally averaged potential energy surfaces for $^{13}C^{16}O_2(v_3)$–He for $v_3 = 0$ and 1. The morphing would be incorporated by multiplying all of the $\overline{R}_e^{\lambda}$ values by the scaling factor $f_{R_e} = 0.99577$, and by multiplying the $\overline{\mathfrak{D}}_e^{\lambda}$ factors for the $v_3 = 1$ surface by the factor $f_{\mathfrak{D}_e}^{[v_3=1]} = 0.99842$.

parameters defining 2D-MLR PES for $^{13}C^{16}O_2(v_3=0)-He$					
$\overline{\mathfrak{D}}_e^0$	32.040	$\overline{R}_e^0$	3.61898	$\overline{\beta}_0^0$	0.0305
$\overline{\mathfrak{D}}_e^2$	−14.790	$\overline{R}_e^2$	0.83646	$\overline{\beta}_0^2$	1.0010
$\overline{\mathfrak{D}}_e^4$	14.617	$\overline{R}_e^4$	−0.26196	$\overline{\beta}_0^4$	−0.0173
$\overline{\mathfrak{D}}_e^6$	−8.050	$\overline{R}_e^6$	0.09368	$\overline{\beta}_1^0$	0.6962
$\overline{\mathfrak{D}}_e^8$	4.315	$\overline{R}_e^8$	−0.03118	$\overline{\beta}_1^2$	0.180
$\overline{\mathfrak{D}}_e^{10}$	−2.135	$\overline{R}_e^{10}$	0.00830	$\overline{\beta}_2^0$	−0.235
$\overline{\mathfrak{D}}_e^{12}$	0.975	$\overline{R}_e^{12}$	−0.00143	$\overline{\beta}_2^2$	−0.203
$\overline{\mathfrak{D}}_e^{14}$	−0.438			$\overline{\beta}_3^0$	0.15
$\overline{\mathfrak{D}}_e^{16}$	0.184				
$\overline{C}_6^0$	72456.88	$\overline{C}_8^0/\overline{C}_6^0$	4.65		
$\overline{C}_6^2$	19135.86	$\overline{C}_8^2/\overline{C}_6^0$	4.85		
parameters defining 2D-MLR PES for $^{13}C^{16}O_2(v_3=1)-He$					
$\overline{\mathfrak{D}}_e^0$	31.982	$\overline{R}_e^0$	3.61997	$\overline{\beta}_0^0$	0.0292
$\overline{\mathfrak{D}}_e^2$	−14.642	$\overline{R}_e^2$	0.83501	$\overline{\beta}_0^2$	1.0006
$\overline{\mathfrak{D}}_e^4$	14.561	$\overline{R}_e^4$	−0.26244	$\overline{\beta}_0^4$	−0.0161
$\overline{\mathfrak{D}}_e^6$	−7.980	$\overline{R}_e^6$	0.09342	$\overline{\beta}_1^0$	0.6914
$\overline{\mathfrak{D}}_e^8$	4.283	$\overline{R}_e^8$	−0.03117	$\overline{\beta}_1^2$	0.178
$\overline{\mathfrak{D}}_e^{10}$	−2.106	$\overline{R}_e^{10}$	0.0081	$\overline{\beta}_2^0$	−0.237
$\overline{\mathfrak{D}}_e^{12}$	0.964	$\overline{R}_e^{12}$	−0.00126	$\overline{\beta}_2^2$	−0.204
$\overline{\mathfrak{D}}_e^{14}$	−0.456			$\overline{\beta}_3^0$	0.15
$\overline{\mathfrak{D}}_e^{16}$	0.193				
$\overline{C}_6^0$	72508.52	$\overline{C}_8^0/\overline{C}_6^0$	4.65		
$\overline{C}_6^2$	19069.74	$\overline{C}_8^2/\overline{C}_6^0$	4.85		

Table A-6. Expansion coefficients $\overline{\mathfrak{D}}_e^{\lambda}$ [cm^{-1}], $\overline{R}_e^{\lambda}$ [Å] and $\overline{\beta}_i^{\lambda}$ defining our unmorphed two-dimensional vibrationally averaged potential energy surfaces for $^{12}C^{18}O_2(v_3)$–He for $v_3 = 0$ and 1. The morphing would be incorporated by multiplying all of the $\overline{R}_e{}^{\lambda}$ values by the scaling factor $f_{R_e} = 0.99577$, and by multiplying the $\overline{\mathfrak{D}}_e^{\lambda}$ factors for the $v_3 = 1$ surface by the factor $f_{\mathfrak{D}_e}^{[v_3=1]} = 0.99842$.

parameters defining 2D-MLR PES for $^{12}C^{18}O_2(v_3=0)$–He					
$\overline{\mathfrak{D}}_e^0$	32.040	$\overline{R}_e^0$	3.61898	$\overline{\beta}_0^0$	0.0305
$\overline{\mathfrak{D}}_e^2$	−14.788	$\overline{R}_e^2$	0.83645	$\overline{\beta}_0^2$	1.0010
$\overline{\mathfrak{D}}_e^4$	14.616	$\overline{R}_e^4$	−0.26196	$\overline{\beta}_0^4$	−0.0173
$\overline{\mathfrak{D}}_e^6$	−8.050	$\overline{R}_e^6$	0.09367	$\overline{\beta}_1^0$	0.6962
$\overline{\mathfrak{D}}_e^8$	4.315	$\overline{R}_e^8$	−0.03119	$\overline{\beta}_1^2$	0.180
$\overline{\mathfrak{D}}_e^{10}$	−2.135	$\overline{R}_e^{10}$	0.00830	$\overline{\beta}_2^0$	−0.235
$\overline{\mathfrak{D}}_e^{12}$	0.975	$\overline{R}_e^{12}$	−0.00142	$\overline{\beta}_2^2$	−0.203
$\overline{\mathfrak{D}}_e^{14}$	−0.438			$\overline{\beta}_3^0$	0.15
$\overline{\mathfrak{D}}_e^{16}$	0.184				
$\overline{C}_6^0$	72457.22	$\overline{C}_8^0/\overline{C}_6^0$	4.65		
$\overline{C}_6^2$	19135.95	$\overline{C}_8^2/\overline{C}_6^0$	4.85		
parameters defining 2D-MLR PES for $^{12}C^{18}O_2(v_3=1)$–He					
$\overline{\mathfrak{D}}_e^0$	31.981	$\overline{R}_e^0$	3.61998	$\overline{\beta}_0^0$	0.0292
$\overline{\mathfrak{D}}_e^2$	−14.640	$\overline{R}_e^2$	0.83499	$\overline{\beta}_0^2$	1.0003
$\overline{\mathfrak{D}}_e^4$	14.560	$\overline{R}_e^4$	−0.26245	$\overline{\beta}_0^4$	−0.0161
$\overline{\mathfrak{D}}_e^6$	−7.979	$\overline{R}_e^6$	0.09342	$\overline{\beta}_0^6$	0.6911
$\overline{\mathfrak{D}}_e^8$	4.282	$\overline{R}_e^8$	−0.03117	$\overline{\beta}_1^0$	0.177
$\overline{\mathfrak{D}}_e^{10}$	−2.105	$\overline{R}_e^{10}$	0.00810	$\overline{\beta}_2^0$	−0.237
$\overline{\mathfrak{D}}_e^{12}$	0.963	$\overline{R}_e^{12}$	−0.00126	$\overline{\beta}_2^2$	−0.204
$\overline{\mathfrak{D}}_e^{14}$	−0.456			$\overline{\beta}_3^0$	0.15
$\overline{\mathfrak{D}}_e^{16}$	0.193				
$\overline{C}_6^0$	72509.52	$\overline{C}_8^0/\overline{C}_6^0$	4.65		
$\overline{C}_6^2$	19062.75	$\overline{C}_8^2/\overline{C}_6^0$	4.85		

Table A-7. Expansion coefficients $\overline{\mathfrak{D}}_e^{\lambda}$ [cm^{-1}], $\overline{R}_e^{\lambda}$ [Å] and $\overline{\beta}_i^{\lambda}$ defining our unmorphed two-dimensional vibrationally averaged potential energy surfaces for $^{13}C^{18}O_2(v_3)$–He for $v_3 = 0$ and 1. The morphing would be incorporated by multiplying all of the $\overline{R}_e^{\lambda}$ values by the scaling factor $f_{R_e} = 0.99577$, and by multiplying the $\overline{\mathfrak{D}}_e^{\lambda}$ factors for the $v_3 = 1$ surface by the factor $f_{\mathfrak{D}_e}^{[v_3=1]} = 0.99842$.

parameters defining 2D-MLR PES for $^{13}C^{18}O_2(v_3=0)$–He					
$\overline{\mathfrak{D}}_e^0$	32.041	$\overline{R}_e^0$	3.61897	$\overline{\beta}_0^0$	0.0305
$\overline{\mathfrak{D}}_e^2$	−14.79	$\overline{R}_e^2$	0.83647	$\overline{\beta}_0^2$	1.001
$\overline{\mathfrak{D}}_e^4$	14.617	$\overline{R}_e^4$	−0.26195	$\overline{\beta}_0^4$	−0.0173
$\overline{\mathfrak{D}}_e^6$	−8.051	$\overline{R}_e^6$	0.09368	$\overline{\beta}_1^0$	0.6962
$\overline{\mathfrak{D}}_e^8$	4.316	$\overline{R}_e^8$	−0.03118	$\overline{\beta}_1^2$	0.18
$\overline{\mathfrak{D}}_e^{10}$	−2.136	$\overline{R}_e^{10}$	0.0083	$\overline{\beta}_2^0$	−0.235
$\overline{\mathfrak{D}}_e^{12}$	0.975	$\overline{R}_e^{12}$	−0.00143	$\overline{\beta}_2^2$	−0.203
$\overline{\mathfrak{D}}_e^{14}$	−0.438			$\overline{\beta}_3^0$	0.15
$\overline{\mathfrak{D}}_e^{16}$	0.184				
$\overline{C}_6^0$	72456.47	$\overline{C}_8^0/\overline{C}_6^0$	4.65		
$\overline{C}_6^2$	19135.75	$\overline{C}_8^2/\overline{C}_6^0$	4.85		
parameters defining 2D-MLR PES for $^{13}C^{18}O_2(v_3=0)$–He					
$\overline{\mathfrak{D}}_e^0$	31.983	$\overline{R}_e^0$	3.61994	$\overline{\beta}_0^0$	0.0293
$\overline{\mathfrak{D}}_e^2$	−14.646	$\overline{R}_e^2$	0.83504	$\overline{\beta}_0^2$	1.0006
$\overline{\mathfrak{D}}_e^4$	14.562	$\overline{R}_e^4$	−0.26242	$\overline{\beta}_0^4$	−0.0162
$\overline{\mathfrak{D}}_e^6$	−7.982	$\overline{R}_e^6$	0.09343	$\overline{\beta}_0^6$	0.6915
$\overline{\mathfrak{D}}_e^8$	4.284	$\overline{R}_e^8$	−0.03117	$\overline{\beta}_1^0$	0.178
$\overline{\mathfrak{D}}_e^{10}$	−2.106	$\overline{R}_e^{10}$	0.00811	$\overline{\beta}_2^0$	−0.237
$\overline{\mathfrak{D}}_e^{12}$	0.964	$\overline{R}_e^{12}$	−0.00127	$\overline{\beta}_2^2$	−0.204
$\overline{\mathfrak{D}}_e^{14}$	−0.456			$\overline{\beta}_3^0$	0.15
$\overline{\mathfrak{D}}_e^{16}$	0.193				
$\overline{C}_6^0$	72507.32	$\overline{C}_8^0/\overline{C}_6^0$	4.65		
$\overline{C}_6^2$	19069.42	$\overline{C}_8^2/\overline{C}_6^0$	4.85		