Rotational Spectrum and Internal Dynamics of Methylpyruvate

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Supporting Information

Completion of the Reference:

[16] GAUSSIAN03, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, **2003**.

Table 1s: Experimental transition frequencies of methylpyruvate.

$J'_{Ka',Kc'} \leftarrow J''_{Ka'',Kc''}$	*species*	*parent*	$^{13}C(1)$	$^{13}C(2)$	$^{13}C(4)$	$^{13}C(7)$
$3_{0,3} \leftarrow 2_{0,2}$	A1	9974.881	9806.846	9931.762	9971.430	9770.774
	E1	9974.753	9806.721	9931.633	9971.303	9770.641
	E2	9974.836	9806.799	9931.715	9971.385	9770.726
	E3	9974.709	9806.676	9931.588	9971.256	9770.604
	E4	9974.709	9806.676	9931.588	9971.256	9770.604
$3_{1,2} \leftarrow 2_{1,1}$	A1	10869.886	10672.785	10817.963	10866.912	10620.928
	E1	10869.642	10672.562	10817.727	10866.675	10620.709
	E2	10869.806	10672.707	10817.886	10866.835	10620.851
	E3	10869.485	10672.402	10817.564	10866.518	10620.533
	E4	10869.649	10672.562	10817.727	10866.675	10620.709
$3_{1,3} \leftarrow 2_{1,2}$	A1	9405.352	9249.054	9365.457	9401.962	9217.311
	E1	9405.317	9249.026	9365.422	9401.998	9217.281
	E2	9405.391	9249.093	9365.492	9401.998	9217.352
	E3	9405.441	9249.149	9365.550	9402.051	9217.407
	E4	9405.278	9248.980	9365.383	9401.894	9217.238
$3_{2,1} \leftarrow 2_{2,0}$	A1	10362.167				
	E1	10356.511				
	E2	10354.822				
	E3	10343.910				
	E4	10361.809				
$3_{2,2} \leftarrow 2_{2,1}$	A1	10168.517				
	E1	10173.901				
	E2	10175.871				
	E3	10186.499				
	E4	10168.599				
$4_{0,4} \leftarrow 3_{0,3}$	A1	13093.185	12879.287	13038.929	13088.287	12837.802
	E1	13093.037	12879.142	13038.780	13088.135	12837.654
	E2	13093.100	12879.205	13038.845	13088.200	12837.725
	E3	13092.946	12879.059	13038.692	13088.049	12837.577
	E4	13092.946	12879.059	13038.692	13088.040	12837.577
$4_{1,3} \leftarrow 3_{1,2}$	A1	14428.117				
	E1	14427.832				
	E2	14428.051				
$4_{1,4} \leftarrow 3_{1,3}$	A1	12489.825	12284.015	12437.460	12485.226	12243.380
	E1	12489.754	12283.949	12437.390	12485.161	12243.312
	E2	12489.716	12284.007	12437.460	12485.226	12243.379
	E3	12489.716	12283.974	12437.390	12485.390	12243.335
	E4	12489.716	12283.919	12437.358	12485.358	12243.282
$4_{2,3} \leftarrow 3_{2,2}$	A1	13519.637				
	E1	13520.536				
	E2	13521.131				
	E3	13524.424				
	E4	13519.468				
$4_{3,2} \leftarrow 3_{3,1}$	A1	13647.771				
	E1	13655.092				
	E2	13655.557				
	E3	13656.156				
	E4	13650.467				
$5_{0,5} \leftarrow 4_{0,4}$	A1	16084.716	15829.200	16020.591	16078.302	15784.726
	E1	16084.553	15829.040	16020.431	16078.140	15784.569
	E2	16084.580	15829.076	16020.463	16078.169	15784.603
	E3	16084.424	15828.903	16020.304	16078.015	15784.446
	E4	16084.424	15828.906	16020.304	16078.015	15784.446
$5_{1,4} \leftarrow 4_{1,3}$	A1	17921.218			17915.360	
	E1	17920.873			17915.541	

	E2	17921.122			17915.169	
	E3	17920.770			17915.407	
	E4	17920.785			17915.015	
$5_{1,5}\leftarrow4_{1,4}$	A1	15539.199			15533.360	
	E1	15539.107			15533.256	
	E2	15539.177			15533.329	
	E3	15539.100			15533.256	
	E4	15539.070			15533.015	
$2_{1,2}\leftarrow1_{0,1}$	A1	9679.883				
	E1	9679.354				
	E2	9679.082				
	E3	9678.386				
	E4	9678.718				
$3_{1,3}\leftarrow2_{0,2}$	A1	12355.427	12214.027	12324.890	12347.732	12228.271
	E1	12354.956	12213.549	12324.427	12347.266	12227.796
	E2	12354.683	12213.291	12324.148	12346.993	12227.531
	E3	12354.129	12212.729	12323.598	12346.441	12226.967
	E4	12354.300	12212.904	12323.768	12346.611	12227.147
$4_{0,4}\leftarrow3_{1,3}$	A1	10712.638				
	E1	10712.829				
	E2	10713.250				
	E3	10713.526				
	E4	10713.352				
$4_{1,4}\leftarrow3_{0,3}$	A1	14870.372				
	E1	14869.958				
	E2	14869.669				
	E3	14869.209				
	E4	14869.317				
$5_{1,5}\leftarrow4_{0,4}$	A1	17316.384				
	E1	17316.035				
	E2	17315.752				
	E3	17315.364				
	E4	17315.441				
$2_{2,0}\leftarrow1_{1,0}$	E1	17493.212				
	E2	17494.924				
	E3	17508.895				
$2_{2,1}\leftarrow1_{1,1}$	E1	17919.295				
	E2	17916.189				
	E3	17899.379				
$3_{2,1}\leftarrow2_{2,1}$	E1	10419.999				
	E2	10423.355				
	E3	10444.571				
$3_{2,2}\leftarrow2_{2,0}$	E1	10110.395				
	E2	10107.341				
	E3	10085.837				
$2_{2,1}\leftarrow2_{1,1}$	E1	10161.746				
	E2	10158.361				
	E3	10140.805				
$2_{2,0}\leftarrow2_{1,2}$	E2	11694.711				
	E3	11709.621				