

Supplementary Information

Detection and characterization of impurities in commercial products with Fourier transform microwave spectroscopy

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Table 1s: Fitting of the average frequencies of the experimental transition frequencies of methyl pyruvate measured as impurity of methyl lactate.

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1  FINAL RESULTS OF          MLAC X righe "b" 2
   A = 5328.651282+- .153714      B = 1939.527434+- .056183
   C = 1450.006535+- .038469      DJ = -.000731+- .000441
   DJK= -.043672+- .013159      DK = .147688+- .040375

*FIXED*      :DDJ= .000000 :DDK= .000000 :
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#	TRANSITION	MEASURED	CALCULATED	DIFFERENCE
1	2 1 2 1 0 1	9678.718	9678.809	-.091
2	3 1 3 2 0 2	12354.300	12354.270	.029
3	4 1 4 3 0 3	14869.317	14869.240	.077
4	5 1 5 4 0 4	17315.441	17315.492	-.051
5	3 0 3 2 0 2	9974.709	9974.753	-.044
6	4 0 4 3 0 3	13092.946	13092.896	.050
7	5 0 5 4 0 4	16084.424	16084.342	.082
8	3 1 3 2 1 2	9405.278	9405.258	.020
9	5 1 5 4 1 4	15539.070	15539.148	-.078
10	4 0 4 3 1 3	10713.352	10713.379	-.026
11	2 2 1 1 1 0	17434.646	17434.729	-.083
12	2 2 0 1 1 1	17973.627	17973.545	.082


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INERTIAL PARAMETERS:
IN. DEF.= -6.87426      IA, IB, IC= 94.84184 260.56816 348.53574
SIGMA = .091           PA, PB, PC= 257.13103 91.40471 3.43713
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