

CSO BROADBAND MOLECULAR LINE SURVEYS I: BENCHMARKING GOBASIC ANALYSIS SOFTWARE

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Motivation for GOBASIC

- Vast broadband datasets from the CSO, ALMA, and the Herschel Space Observatory

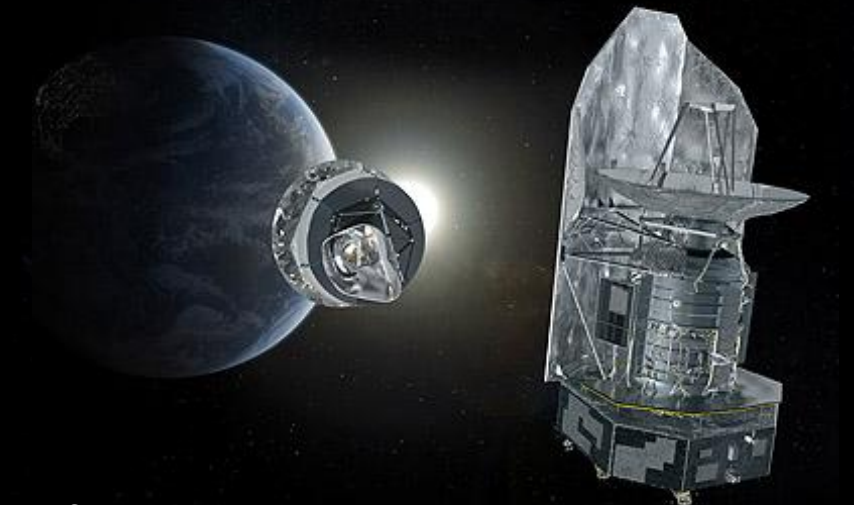
Smallest CSO dataset ~ 30 GHz of data,
32 surveys now on hand



ESO/B. Tafreshi (twanight.org)



Jacob C. Laas

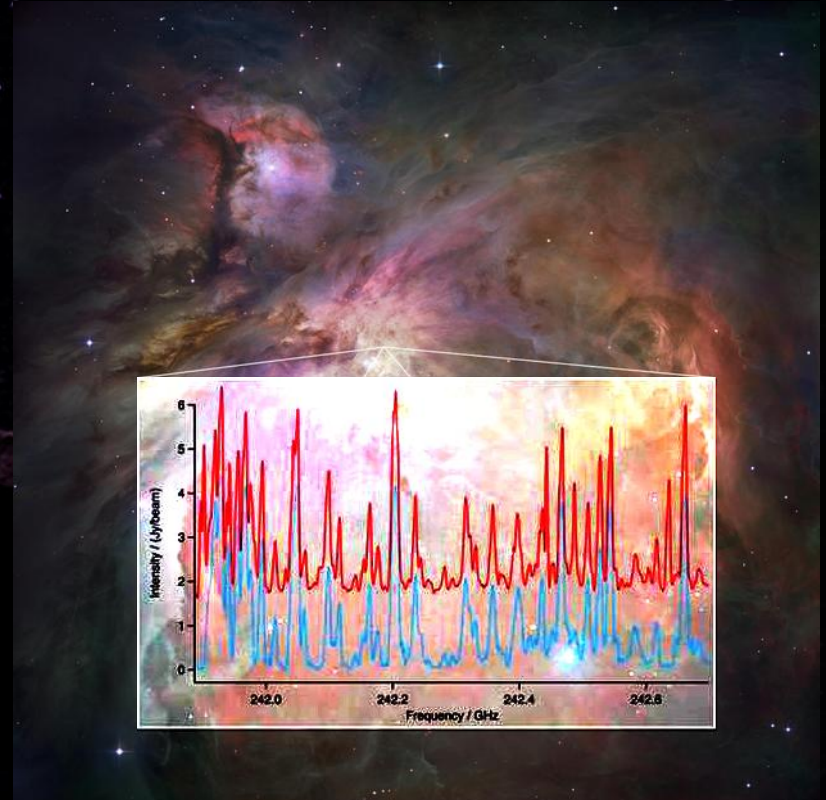


ESA

Motivation for GOBASIC

- Probed sources with many complex molecules and many components of gas

Increased sensitivity leads to line dense spectra with complex line blending



ALMA ethyl cyanide overlay on Orion spectrum. Fortman, et al., NRAO/AUI/NSF, NASA

Approach of GOBASIC

Time required for analysis

- Import JPL/CDMS catalogs with no special formatting required
- Little user input necessary
- Fast global, derivative-free pattern search optimization
- Parallel processing capabilities
- LTE assumptions

Complexity of Analysis

- Global analysis
- Simultaneous multi-molecule, multi-component fitting up to four components
- Iterative analysis procedure

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TextPad - C:\Users\widiuslabuser\Desktop\GOBASIC\CH3OH.cat

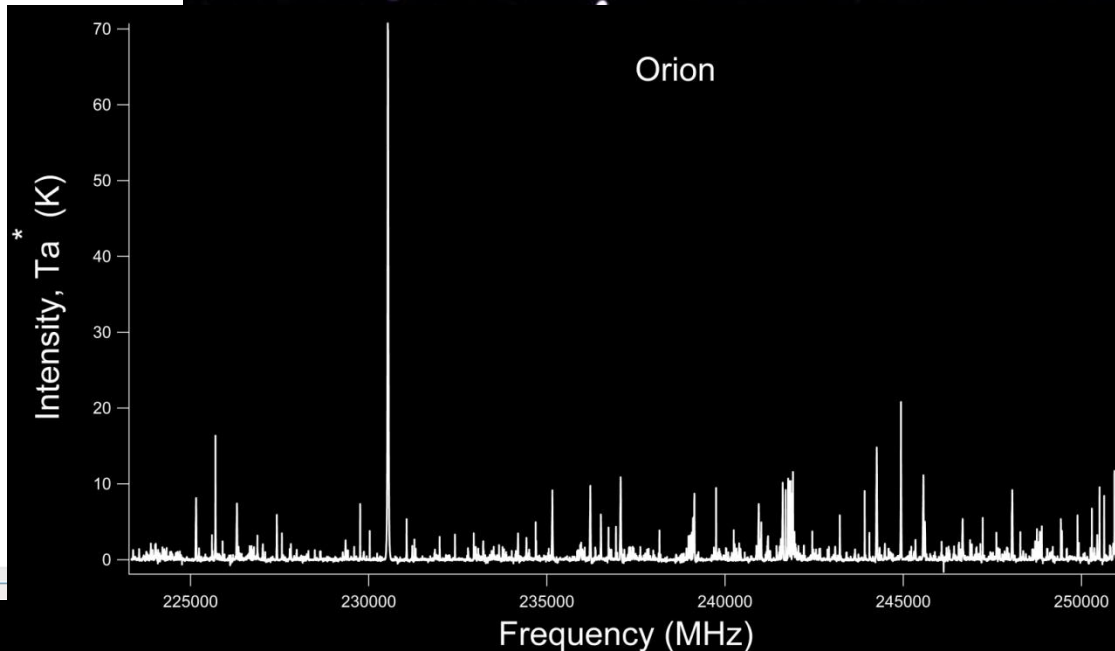
File Edit Search View Tools Macros Configure Window Help

Find incrementally Match case

CH3OH.cat

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902.201	0.125	-12.5670	3	1404.3200	75	32003130437	3m	1		37	3	p	1
953.339	0.340	-16.6502	3	991.5550	43	32003130421	1s	1		22a3	s		0
962.347	0.006	-10.1400	3	242.1430	9	320031304	4	1m	1	4	1	p	1
982.301	0.174	-17.8172	3	464.3000	9	320031304	4-2s	2		5-5	s	2	
991.369	0.003	-9.8234	3	310.3570	37	32003130418	3m	0		18	3	p	0
1020.184	0.004	-10.6167	3	710.2530	57	32003130428	4p	0		28	4	p	0
1038.991	0.153	-12.5812	3	1465.2100	77	32003130438	3m	1		38	3	p	1
1049.700	0.022	-16.2963	3	406.9910	43	32003130421	3p	0		22	0	p	0
1061.006	0.025	-10.5470	3	513.0370	39	32003130419	3m	1		19	3	p	1
1092.070	0.016	-10.4081	3	484.1850	7	320031304	3	1m	2	3	1	p	2
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1482.224	0.345	-12.3945	3	861.5910	35	32003130417	4s	2		18	5	s	2
1566.361	0.035	-10.3693	3	578.8670	43	32003130421	2m	1		21	2	p	1
1616.593	0.004	-9.3029	3	132.6570	23	32003130411	2p	0		11	2	p	0
1670.411	0.019	-9.1000	3	542.2270	45	32003130422	6m	0		21	7	p	0
1670.425	0.019	-9.1000	3	542.2270	45	32003130422	6p	0		21	7	p	0
1728.190	0.009	-10.3803	3	805.2490	61	32003130430	4p	0		30	4	p	0
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1836.686	0.005	-9.4466	3	373.1970	41	32003130420	3m	0		20	3	p	0
1877.354	0.040	-10.2956	3	614.1780	45	32003130422	2m	1		22	2	p	1
2019.508	0.013	-9.7080	3	259.8250	13	320031304	6	1m	1	6	1	p	1
2216.303	0.012	-10.2792	3	855.1500	63	32003130431	4p	0		31	4	p	0
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2260.312	0.006	-9.0970	3	151.9990	25	32003130412	2p	0		12	2	p	0
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2647.270	0.990	-11.0022	3	1527.6390	79	32003130435	3m	1		38	4	p	1
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2729.090	0.040	-9.8372	3	498.6230	11	320031304	5	1m	2	5	1	p	2
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3077.467	0.008	-8.9157	3	172.9480	27	32003130413	2p	0		13	2	p	0
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3205.301	0.007	-9.1309	3	442.4590	45	32003130422	3m	0		22	3	p	0
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3343.669	0.089	-9.3550	3	1072.5550	65	32003130432	8p	0		33	7	p	0
3343.735	0.089	-9.3550	3	1072.5550	65	32003130432	8m	0		33	7	p	0
3387.356	0.013	-12.6449	3	25.1410	9	320031304	4	0s	0	3	2	s	0
3458.655	0.021	-9.4255	3	283.9330	17	320031304	6	1m	1	8	1	p	1
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3596.753	0.069	-10.0893	3	771.3700	53	32003130426	2m	1		26	2	p	1

Input deconvolved observational data and JPL/CDMS catalog



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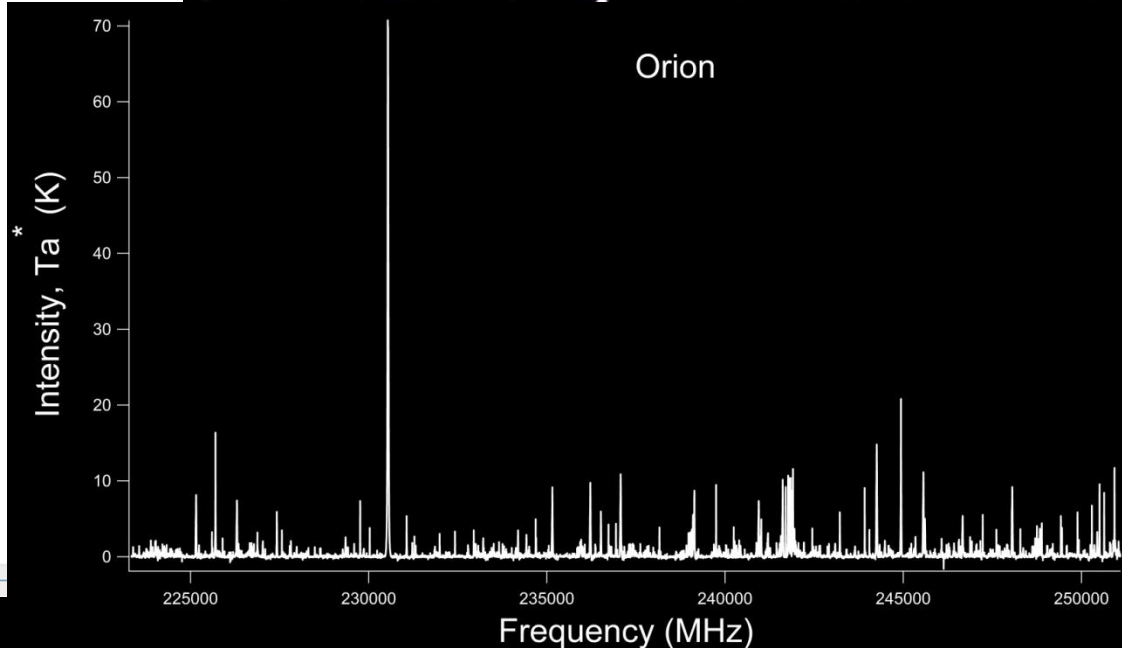
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953.339	0.340	-16.6502	3	991.5550	43	32003130421	1s	1		22a3	s	0	
962.347	0.006	-10.7400	3	242.1430	9	320031304	4	1m	1	4	1	p	1
982.301	0.174	-17.8172	3	464.3000	9	320031304	4-2s	2		5-5	s	2	
991.369	0.003	-9.8234	3	310.3570	37	32003130418	3m	0		18	3	p	0
1020.184	0.004	-10.6129	3	710.2530	57	32003130429	4p	0		28	3	p	0
1038.991	0.153	-12.5812	3	1465.2100	77	32003130438	3m	1		38	3	p	1
1049.700	0.022	-16.2963	3	406.9910	43	32003130421	3p	0		22	0	p	0
1061.006	0.025	-10.5470	3	513.0370	39	32003130419	3m	0		19	2	p	1
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1120.370	0.003	-9.5370	3	114.9230	21	32003130410	2p	0		10	2	m	0
1190.530	0.187	-12.6026	3	1527.6880	79	32003130439	5s	1		39	5	s	1
1211.477	0.024	-9.5972	3	740.2030	57	32003130428-5s	0			27-6	s	0	
1275.477	0.298	-13.5934	3	1167.6130	75	32003130437	3m	0		36	5	m	0
1295.417	0.030	-10.4529	3	545.1530	41	32003130429	4p	1		29	4	p	1
1334.617	0.006	-10.4927	3	756.9500	59	32003130429	4p	0		29	4	p	0
1357.576	0.228	-12.6310	3	1591.7500	81	32003130440	3m	1		40	3	p	1
1360.515	0.004	-9.6268	3	340.9740	39	32003130419	3m	0		19	2	p	1
1397.297	0.905	-11.5572	3	1527.6410	79	32003130439	3p	1		38	4	p	1
1443.060	0.009	-9.8995	3	250.1800	11	320031304	5	1m	1	5	1	p	1
1482.224	0.345	-12.3945	3	861.5910	35	32003130417	4s	2		18	5	s	2
1566.361	0.035	-10.3693	3	578.8670	43	32003130421	2m	1		21	2	p	1
1616.593	0.004	-9.3029	3	132.6570	23	32003130411	2p	0		11	2	m	0
1670.411	0.019	-9.1000	3	542.2270	45	32003130422	6m	0		21	7	m	0
1670.425	0.019	-9.1000	3	542.2270	45	32003130422	6p	0		21	7	p	0
1728.190	0.009	-10.3803	3	805.2490	61	32003130430	4p	0		30	4	p	0
1819.795	0.027	-10.0875	3	490.6020	9	320031304	4	1m	2	4	1	p	2
1836.686	0.005	-9.4466	3	373.1970	41	32003130420	3m	0		20	3	p	0
1877.354	0.040	-10.2956	3	614.1780	45	32003130422	2m	1		22	2	p	1
2019.508	0.013	-9.7080	3	259.8250	13	320031304	4	1m	1	6	1	p	1
2216.303	0.012	-10.2792	3	855.1500	63	32003130431	4p	0		31	4	m	0
2232.047	0.046	-10.2312	3	651.0850	47	32003130423	2m	1		23	2	p	1
2260.312	0.006	-9.0970	3	151.9990	25	32003130412	2p	0		12	2	p	0
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2328.191	40.080	-11.8790	3	2068.5460	69	3200313043414p	2			3515	m	1	
2442.865	0.006	-9.2816	3	407.0260	43	32003130421	3m	0		21	3	p	0
2502.768	0.001	-8.5596	3	14.9040	5	320031304	2	1m	0	2	1	p	0
2558.441	48.143	-14.0387	3	2257.5300	75	3200313043715m	2			3617	p	1	
2558.441	48.143	-14.0387	3	2257.5300	75	3200313043715p	2			3617	m	1	
2581.415	0.023	-9.0951	3	489.1960	27	32003130413-6s	1			12-7	s	1	
2634.222	0.053	-10.1756	3	689.5870	49	32003130424	2m	1		24	2	p	1
2647.270	0.090	-11.0022	3	1527.6390	79	32003130439	3m	1		38	4	m	1
2691.462	0.017	-9.5527	3	271.0760	15	320031304	7	1m	1	7	1	p	1
2710.160	0.038	-8.4415	3	695.9520	47	32003130423	4s	1		22	3	s	1
2729.090	0.040	-9.8372	3	498.6230	11	320031304	5	1m	2	5	1	p	2
2816.374	0.018	-10.1888	3	906.6510	65	32003130432	4p	0		32	4	m	0
2827.172	0.127	-10.2690	3	999.0150	59	32003130429	5s	1		30	4	s	1
2864.044	4.825	-14.3834	3	1580.5040	61	3200313043013s	1			3115	s	0	
2925.982	0.014	-7.9885	3	121.8990	23	32003130411	2s	0		10	3	s	0
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3077.467	0.008	-8.9157	3	172.9480	27	32003130413	2p	0		13	2	m	0
3087.783	0.060	-10.1284	3	729.6820	51	32003130425	2m	1		25	2	p	1
3205.301	0.007	-9.1309	3	442.4590	45	32003130422	3m	0		22	3	p	0
3279.976	0.007	-8.2280	3	218.5680	9	320031304	4	1s	1	3	0	s	1
3289.936	0.873	-15.5850	3	803.5390	29	3200313041410s	1			15	7	s	2
3343.669	0.089	-9.3550	3	1072.5550	65	32003130432	8p	0		33	7	m	0
3343.735	0.089	-9.3550	3	1072.5550	65	32003130432	8m	0		33	7	m	0
3387.356	0.013	-12.6449	3	25.1410	9	320031304	4	0s	0	3	2	s	0
3459.655	0.021	-9.4555	3	283.9300	17	320031304	3	1m	1	8	3	m	1
3460.655	0.093	-11.4595	3	865.3560	63	32003130431	4s	0		32	2	s	0
3513.312	1.794	-12.4744	3	1377.3750	57	3200313042812m	1			2914	p	0	
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3547.921	0.025	-10.1088	3	959.7520	67	32003130433	4p	0		33	4	m	0
3596.753	0.069	-10.0893	3	771.3700	53	32003130426	2m	1		26	2	p	1

Input deconvolved observational data and JPL/CDMS catalog



- Internal selection of catalog data for line intensity and uncertainty limits
- Internal calibration of observational data for telescope efficiency and beam dilution

Approach of GOBASIC

Time required for analysis

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- Parallel processing capabilities
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LTE population diagram equations from Goldsmith and Langer (1999) *ApJ* **517** used to simulate spectra:

$$T_a = \frac{hc^3 N_T A_{ul} g_u e^{-E_u/kT}}{8\pi k \nu^2 \Delta \nu Q(T)} \left(\frac{1 - e^{-\tau}}{\tau} \right)$$

$$\tau = \frac{N_T}{Q(T)} \frac{c^3}{\Delta \nu 8\pi \nu^3} A_{ul} g_u e^{-E_u/kT} \left(e^{h\nu/kT} - 1 \right)$$

Pattern search optimization to minimize difference between simulated spectrum and observational spectrum:

$$f(N_T, (m, c, i), \Delta \nu(m, c, i), T(m, c, i), v(m, c, i)) = ||\text{obs}(\nu) - T_{\text{spec}}(\nu)||$$

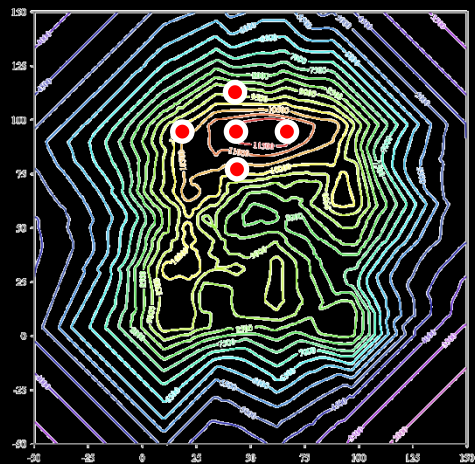
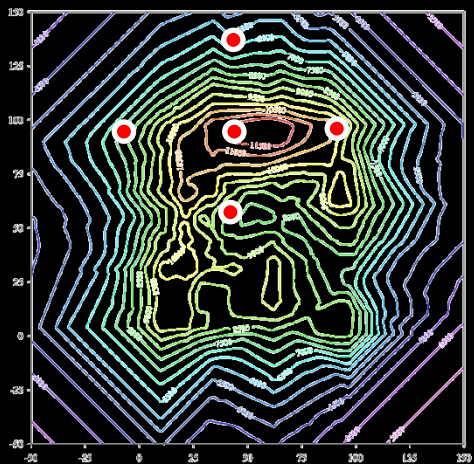
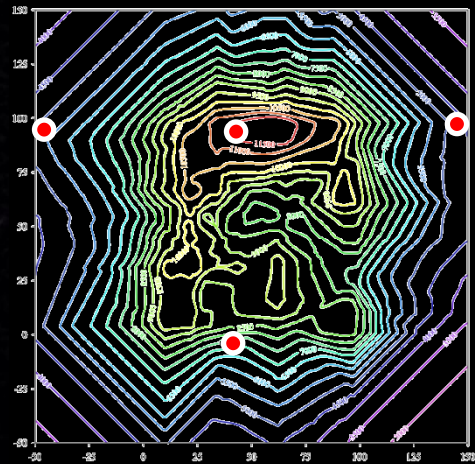
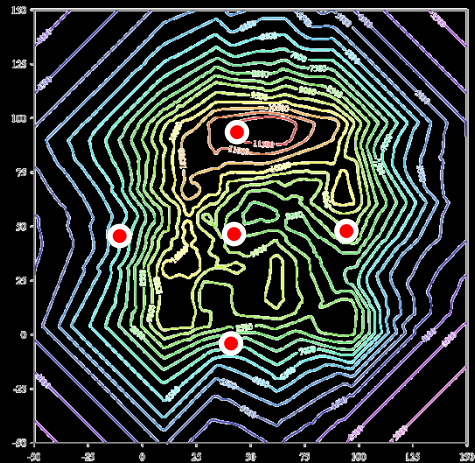
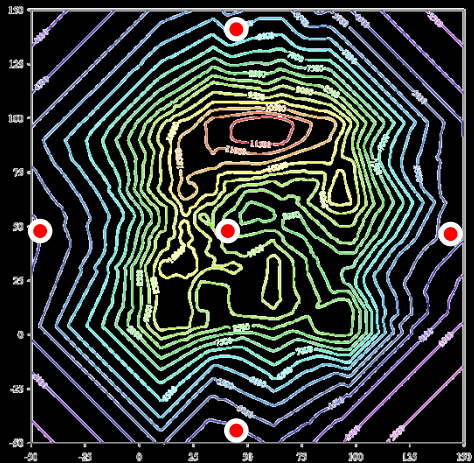
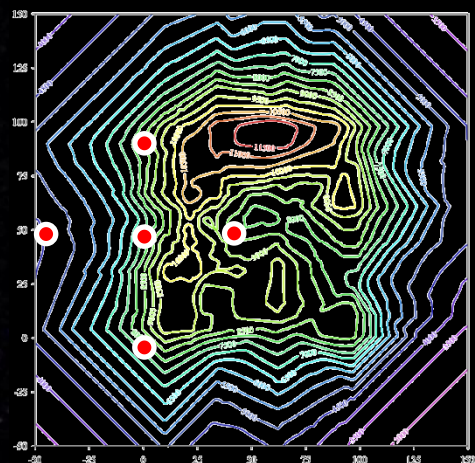
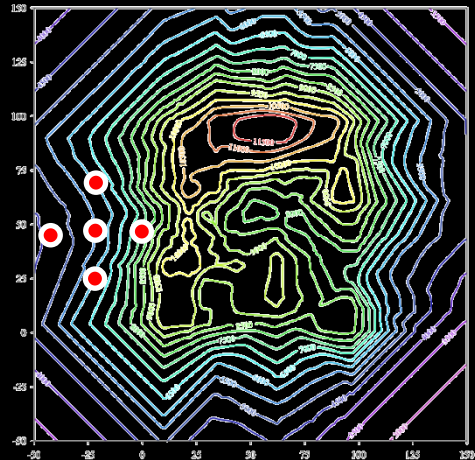
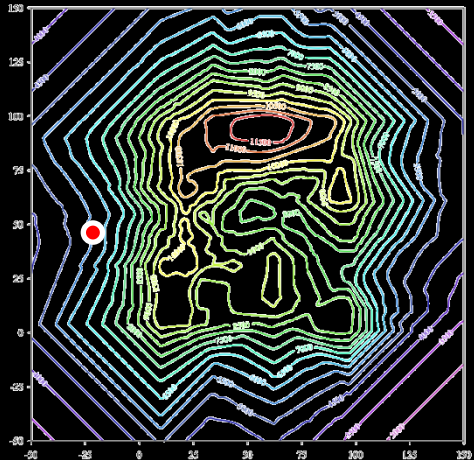
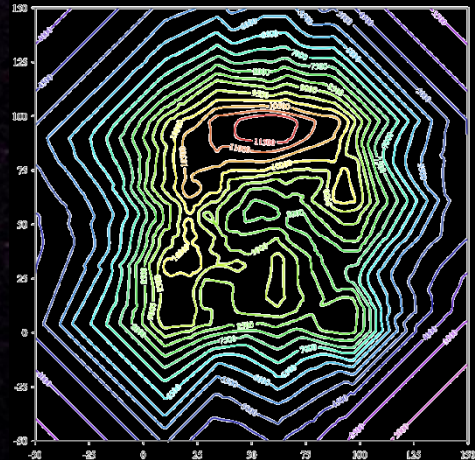
Approach of GOBASIC

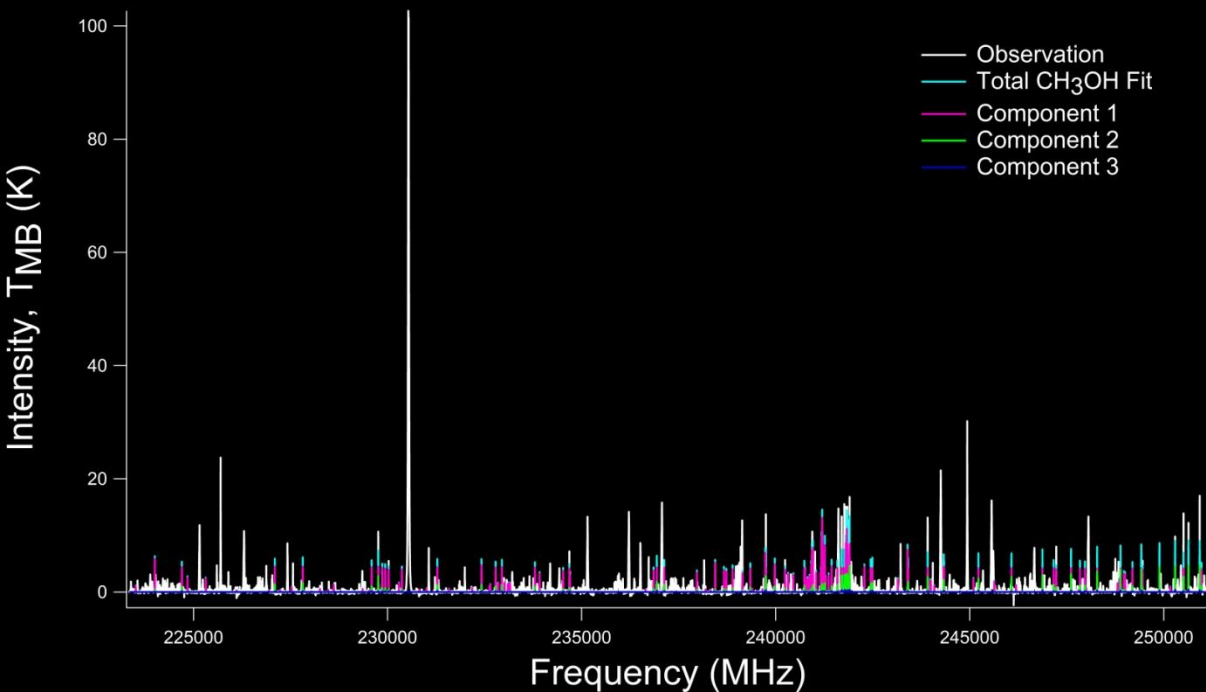
Time required for analysis

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- Little user input necessary
- Fast global, derivative-free pattern search optimization
- Parallel processing capabilities
- LTE assumptions

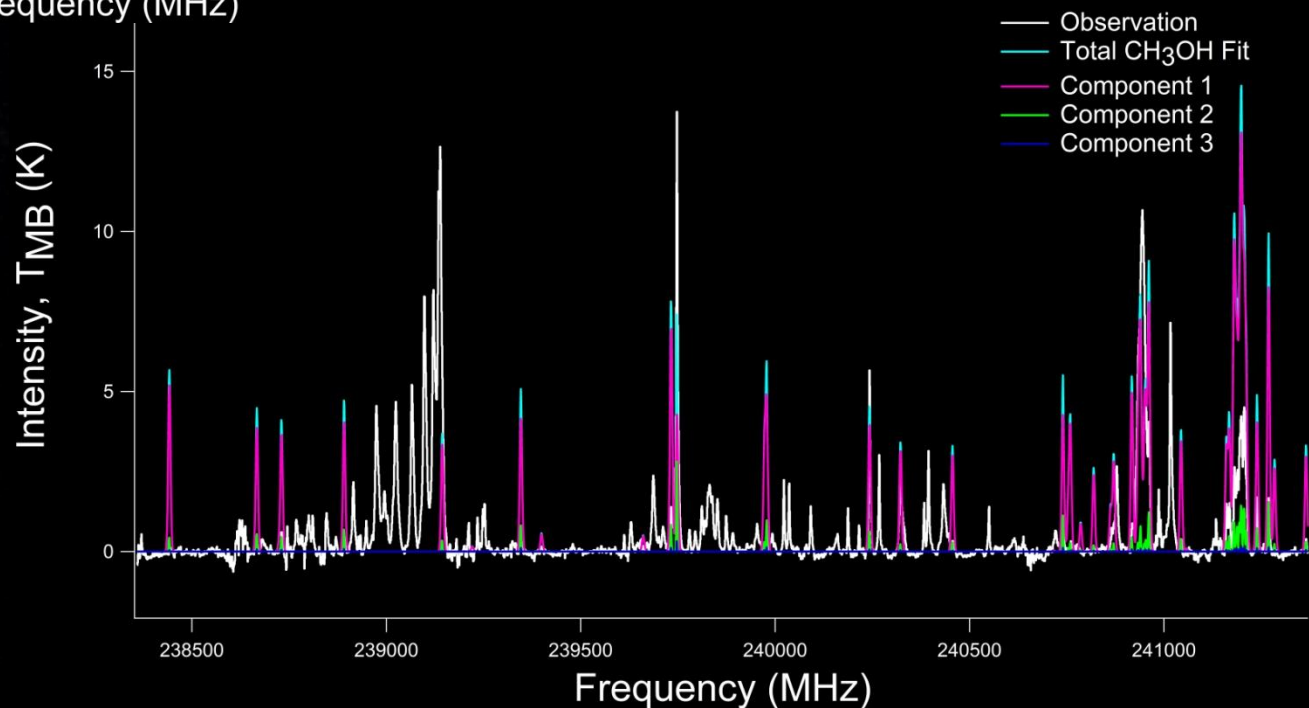
Complexity of Analysis

- Global analysis
- Simultaneous multi-molecule, multi-component fitting up to four components
- Iterative analysis procedure





Output figures show
best fit simulations
for each component
and total simulated
spectrum



TextPad - C:\Users\widiuslabuser\Desktop\Orion\CH3OH_1Results.csv

```
File Edit Search View Tools Macros Configure Window Help
[Icons] Find incrementally
CH3OH_1Results.csv
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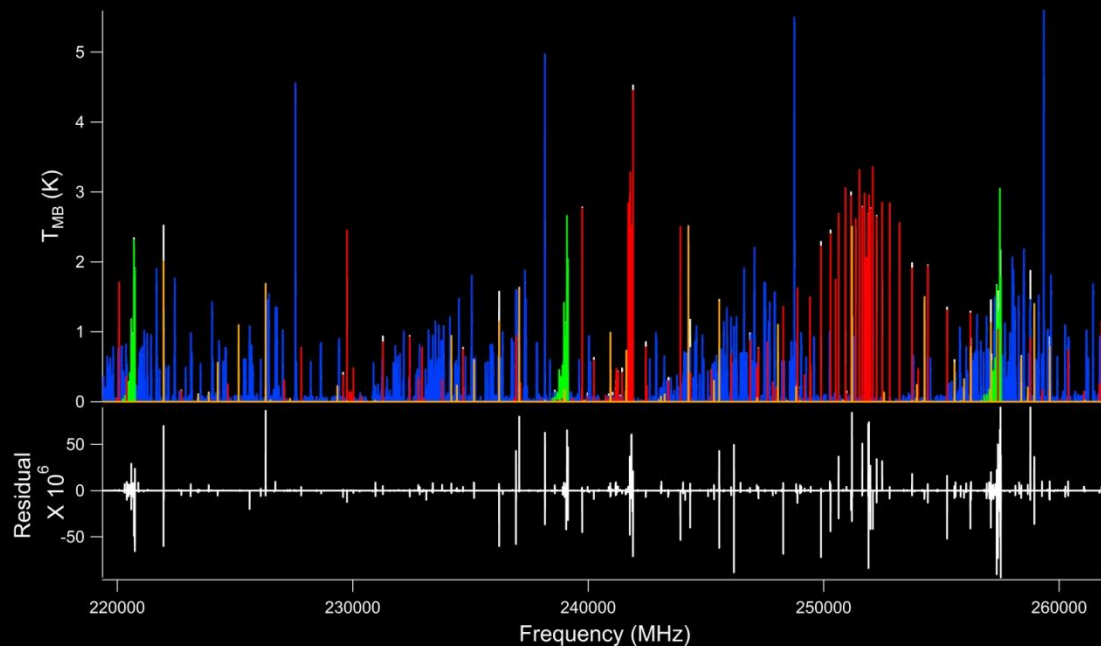
For Help, press F1 1

Output files in .csv format include best fit variables with associated errors and simulated spectra for each component

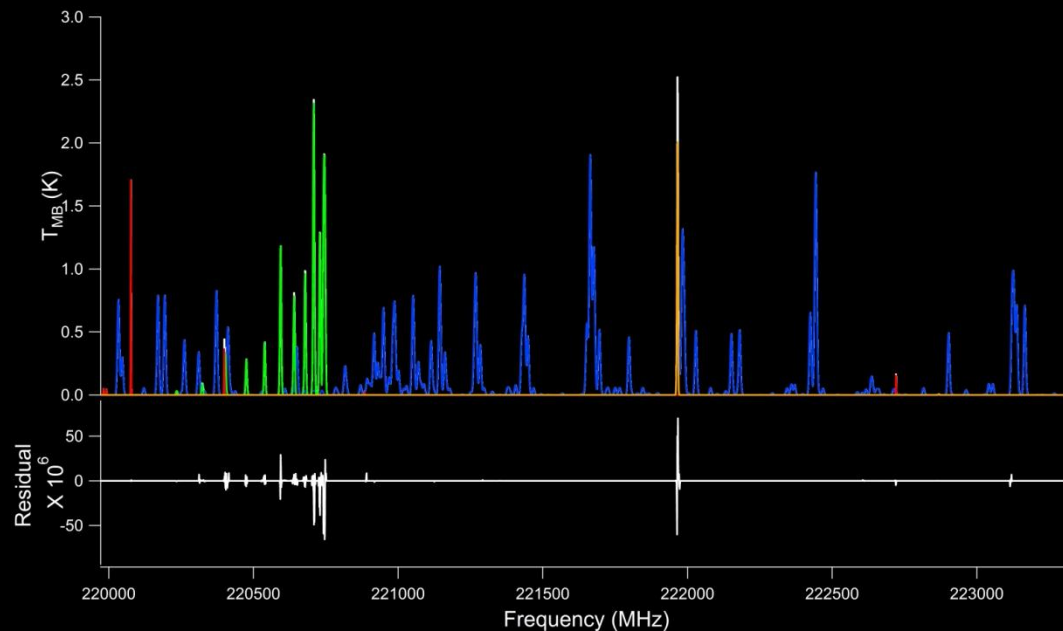
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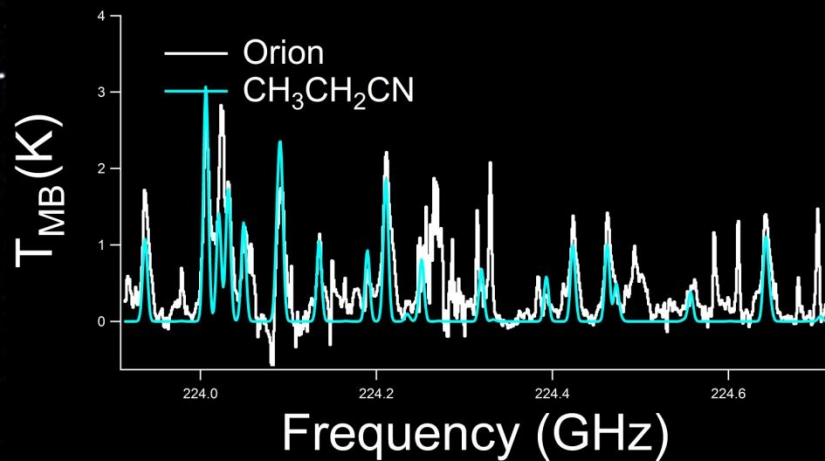
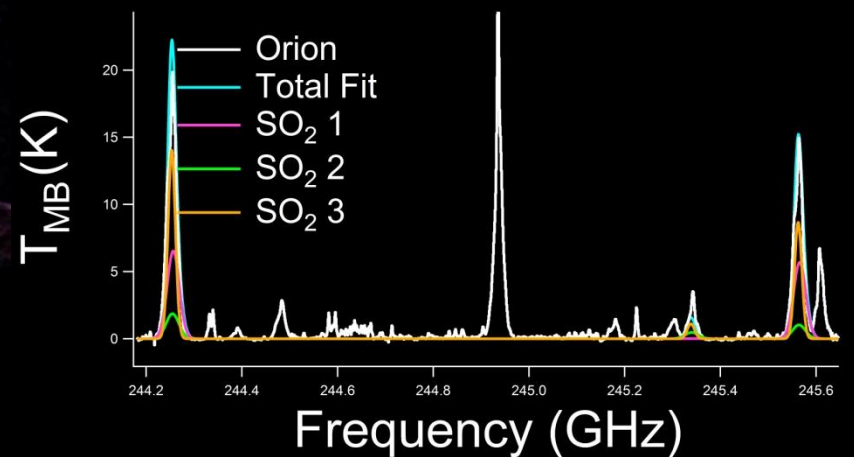
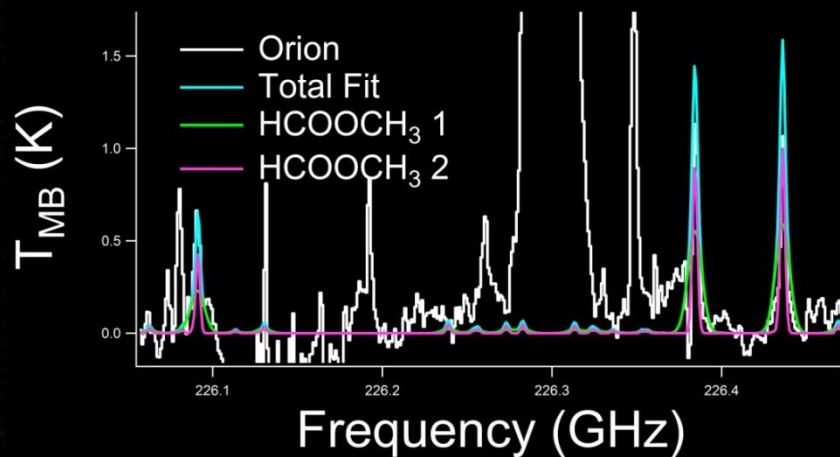
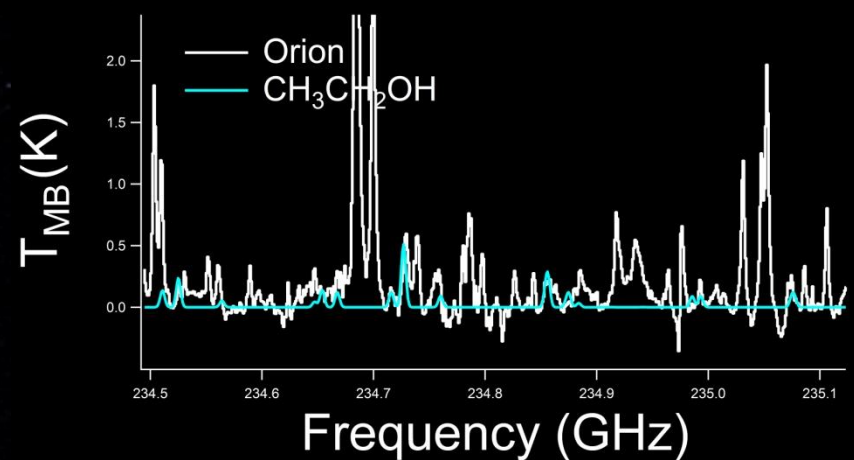
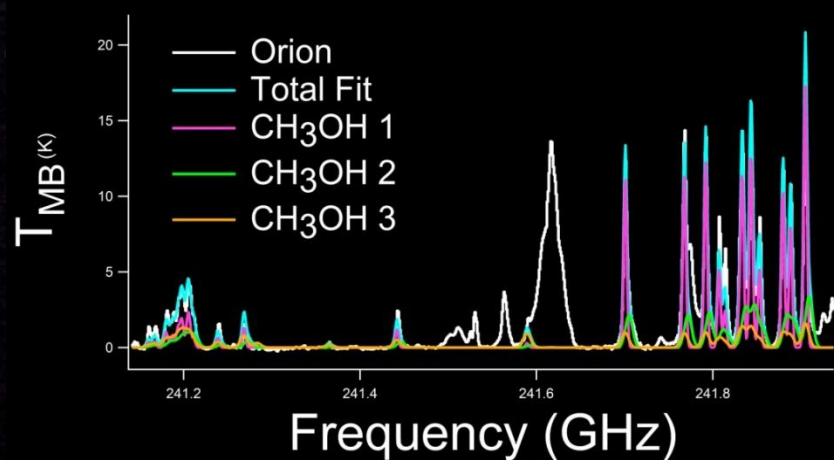
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[Icons] Find incrementally
CH3OH_1Fit.csv
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For Help, press F1 1 1 Read Ovr Block Sync Rec Caps



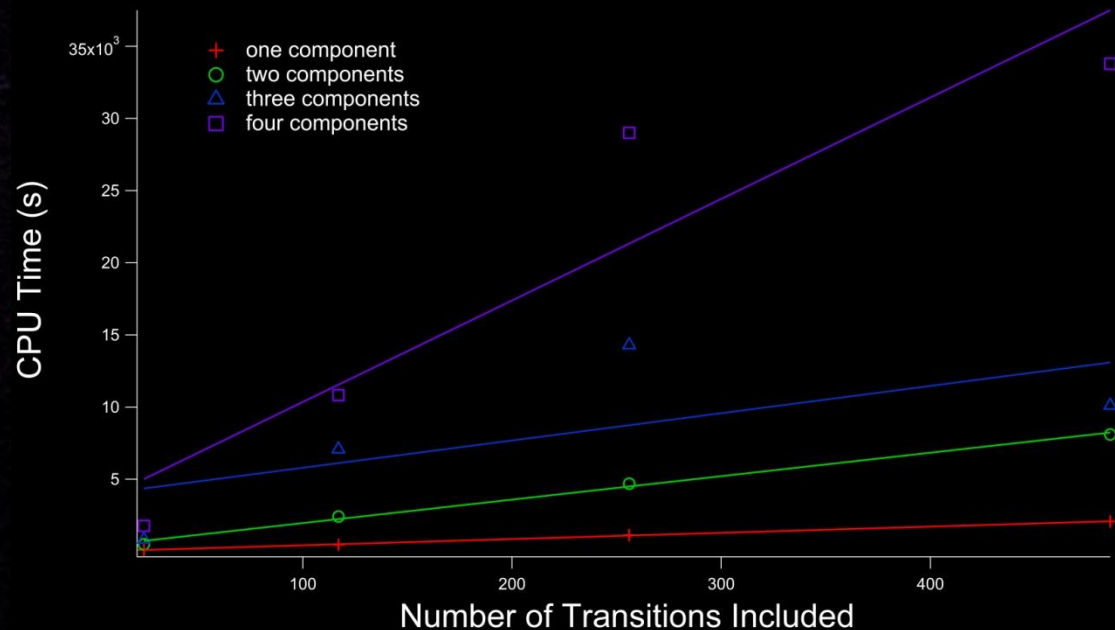
Noiseless simulated spectral fit test. Six molecule spectrum simulated. Residual multiplied by 10^6 as to be visible.



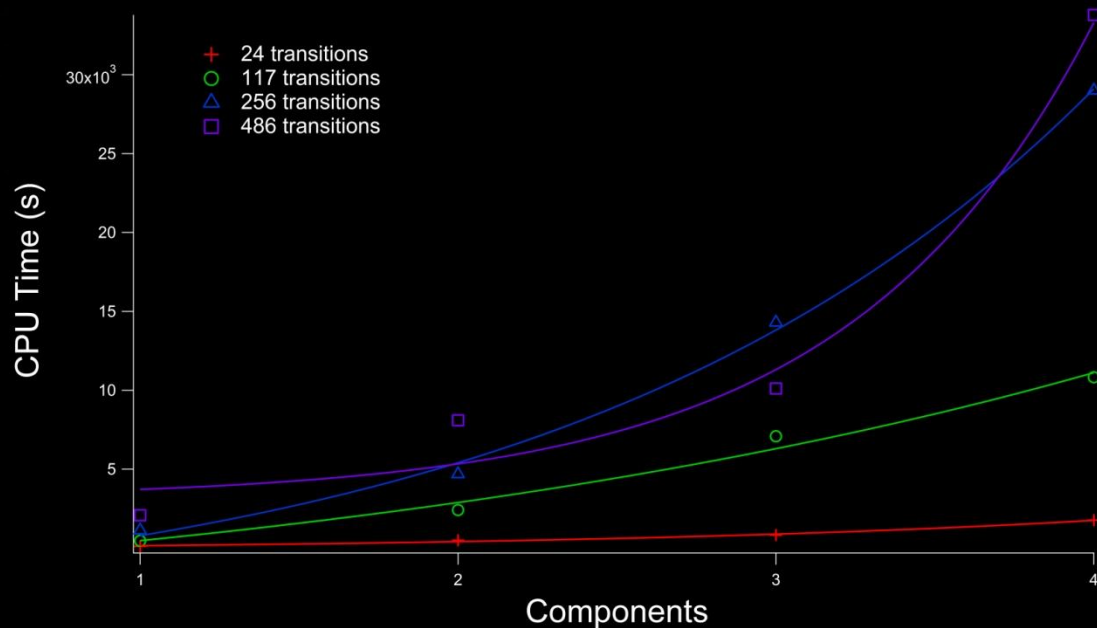


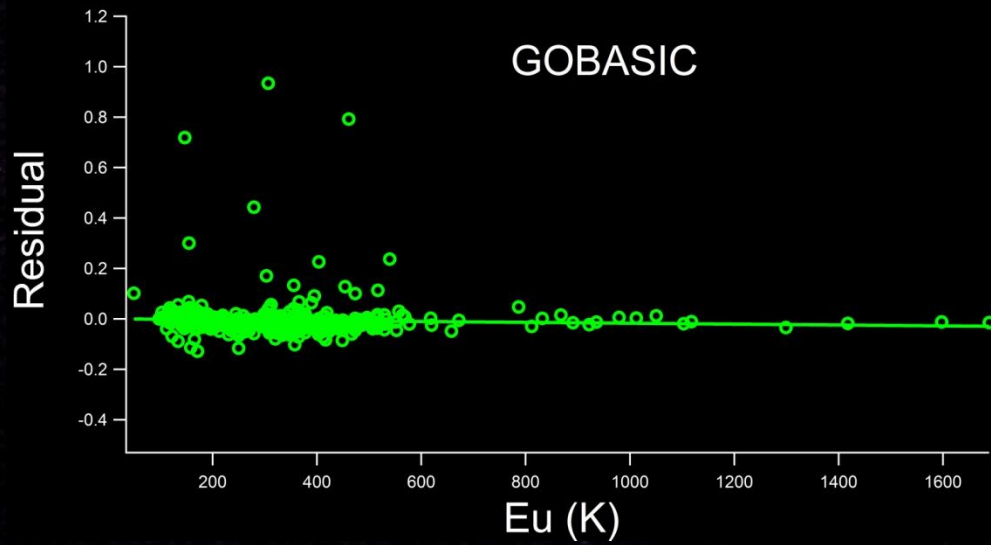
- Fit test on Orion showed good match to observational data and to previous analysis of Orion of Blake et al. 1986 *ApJS* 60.

Time benchmarking trials used CH₃OH analysis on Orion broadband line survey



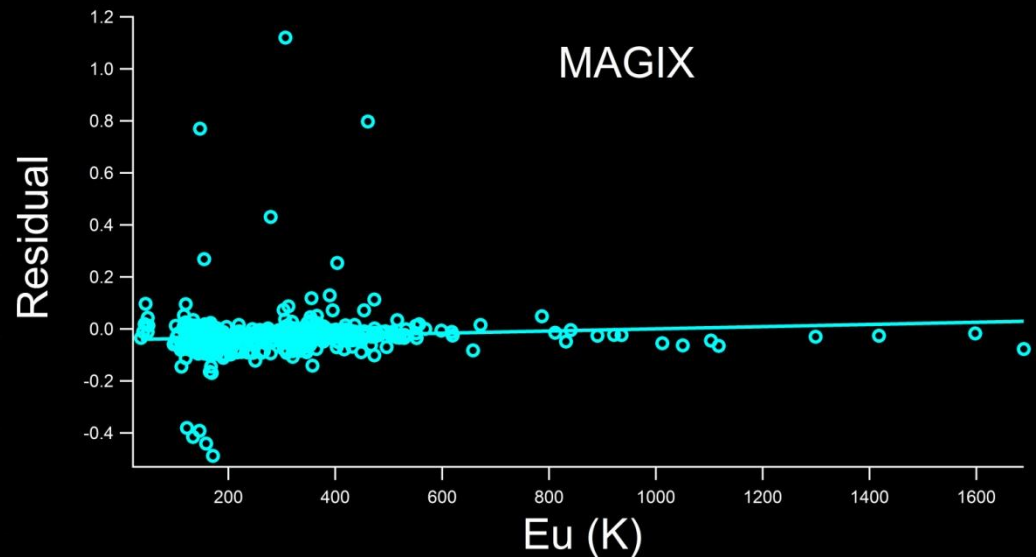
$$\text{CPU time} \sim 7(\text{trans}) + 150e^{1.3(\text{components})}$$





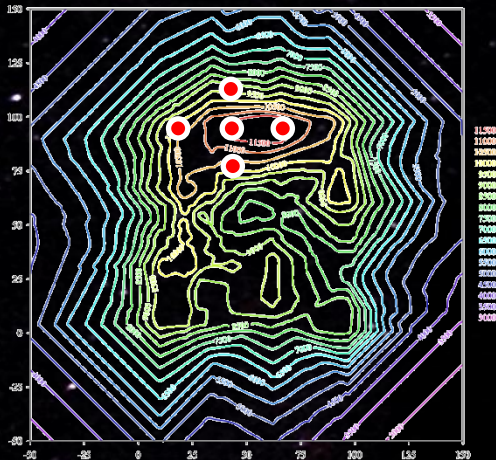
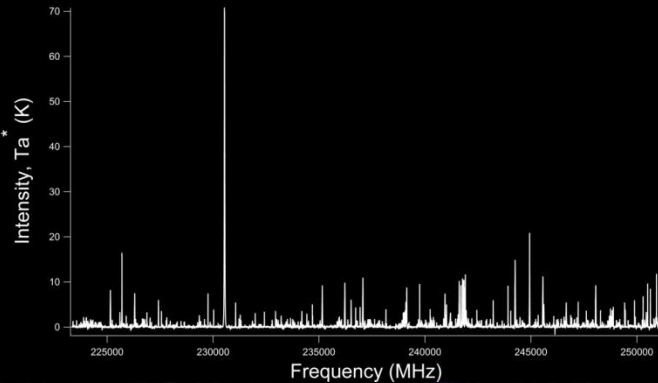
Single component methyl formate fit on CSO survey of W3. Comparison of residual vs upper state energy. Positive residual is under prediction, negative residual is over prediction.

Over prediction of lower E_u (K) lines with MAGIX results in skewing toward lower temperatures.



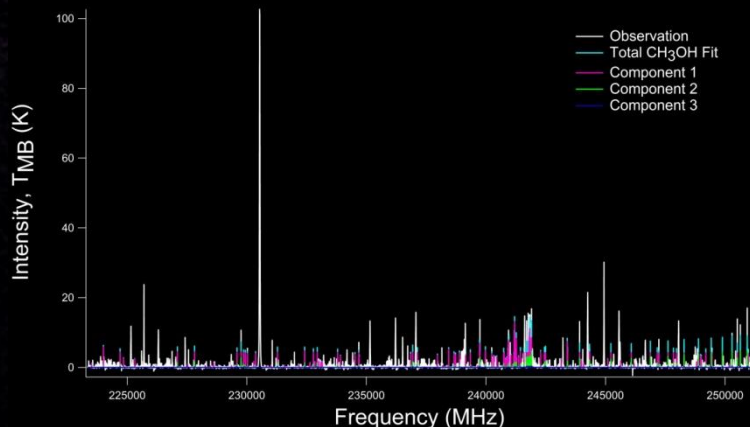
Summary

- GOBASIC analysis is fast, robust, and easy with little data calibration and user input required.



Summary

- Final results are provided conveniently as graphs, simulation files, and tables of best fit parameters.



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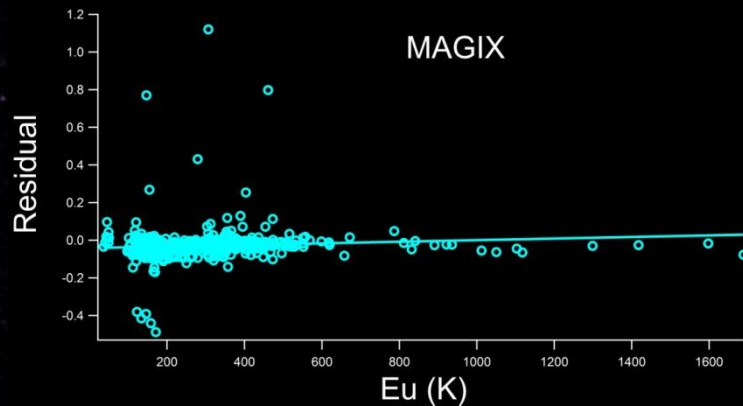
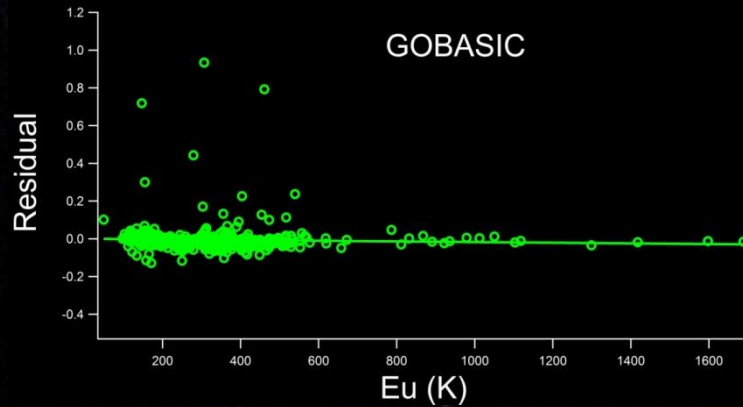
TextPad - C:\Users\widi\labuser\Desktop\Orion\CH3OH_1Fit.csv
File Edit Search View Tools Macros Configure Window Help
CH3OH_1Fit.csv
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229605.0 0.5 92878775e-323.5 92878775e-323
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229617.0 0.4 612439339e-275.4 612439339e-275
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229635.0 0.2 091588902e-210.2 091588902e-210
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229637.0 0.9 339473504e-204.9 339473504e-204
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```

```

TextPad - C:\Users\widi\labuser\Desktop\Orion\CH3OH_1Results.csv
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7.883122627e+16,4.829160927e+23,12.73511391,2.300.8887788,1.053532527e-05,-2.177426336
  
```

Summary

- Compared to MAGIX and rotation diagram analysis, GOBASIC is less susceptible to skewed results from incorrect line shape analysis.



Future Work

- Complete Analysis of CSO and HIFI surveys (James Sanders T107)
- Expand use of GOBASIC beyond Widicus Weaver lab (Paper submitted to ApJS)

Acknowledgements

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Jonas Zmuidzinas, Frank Rice, Geoffrey Blake, CSO
Staff

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1428755

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Grant

