

## Electronic Supplementary Material for:

# Can Calculated Harmonic Vibrational Spectra Rationalize the Structure of TiC-based Nanoparticles?

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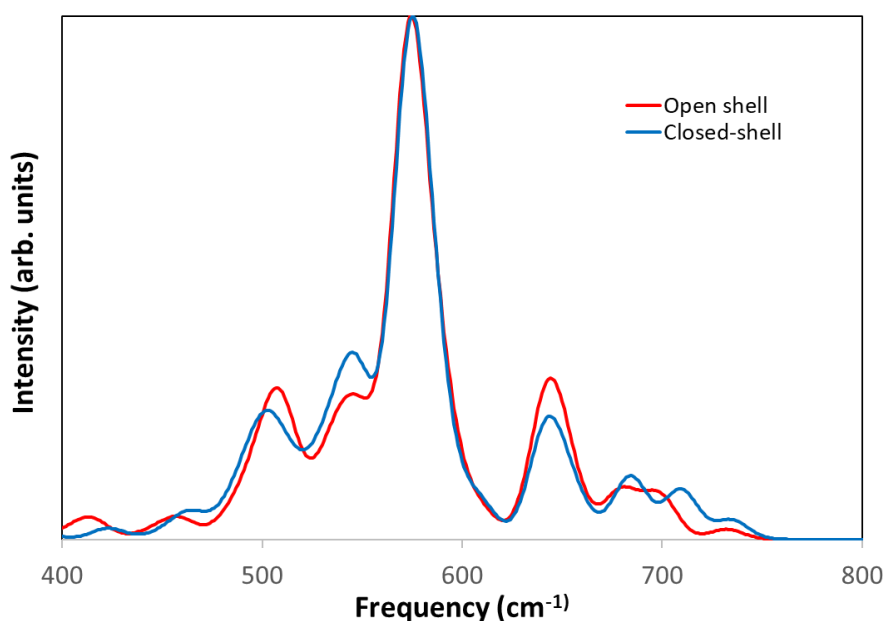
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1. DFT-calculated IR spectra (PBE) for the  $\text{Ti}_{17}\text{C}_{18}$  NP based on a rocksalt cut  $\text{Ti}_{18}\text{C}_{18}$  NP with one corner Ti atom removed with: i) an open shell electronic structure (2 unpaired electrons), ii) a closed shell electronic structure.



2. Tables of calculated harmonic frequencies and corresponding intensities for all reported spectra.

**Ti<sub>14</sub>C<sub>13</sub>**

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
10.419	3.96E-06
10.431	1.45E-06
161.006	3.04E-05
161.161	2.48E-06
181.858	1.06E-05
182.230	7.60E-07
182.578	4.52E-06
205.803	6.89E-02
205.866	6.87E-02
206.046	6.83E-02
211.940	1.96E-06
212.036	1.07E-05
212.163	2.78E-05
232.421	1.47E-05
232.639	4.62E-06
232.713	3.50E-05
252.221	1.45E-05
252.514	7.78E-06
269.089	1.15E-04
291.264	2.25E-04
291.346	3.42E-04
291.618	8.96E-05
298.214	3.65E-04
298.538	1.18E-04
304.534	4.90E-01
304.734	4.65E-01
304.790	4.73E-01
310.159	1.10E-04
310.329	1.52E-04
310.361	4.43E-04
324.293	1.56E+00
324.788	1.58E+00
325.010	1.58E+00
338.765	8.23E-04
351.778	2.16E-04
351.865	3.64E-05
351.974	1.15E-04
370.589	1.74E-04
382.733	9.97E-06
407.696	1.88E-04
407.866	1.07E-04
408.085	4.29E-05
424.427	1.02E-02
424.575	1.20E-02

424.674	1.07E-02
428.729	8.26E-05
428.780	1.38E-04
428.973	6.69E-05
444.918	5.98E-05
445.200	2.29E-05
445.688	5.24E-05
482.714	2.33E-03
482.898	1.29E-03
483.254	4.13E-04
493.256	3.90E+00
493.704	3.91E+00
494.005	3.90E+00
513.606	7.44E-04
513.648	8.57E-04
555.132	1.07E-04
555.360	1.20E-04
556.094	4.40E-05
557.387	5.23E-05
558.188	2.81E-04
588.004	1.45E-04
669.968	6.97E+00
670.067	6.98E+00
670.537	6.98E+00
698.688	1.33E-01
699.000	1.23E-01
699.341	1.29E-01
740.808	1.27E-05
740.920	9.04E-05
741.214	6.43E-05
792.713	7.56E-05

**(TiC)<sub>18</sub>**

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
127.514	3.47E-09
148.637	9.53E-03
148.665	9.55E-03
185.837	3.44E-03
185.912	3.46E-03
191.562	6.62E-07
195.425	3.59E-02
207.983	4.95E-08
209.683	4.53E-08
214.623	6.54E-03
214.624	6.54E-03
220.703	2.20E-08
224.966	8.96E-09
234.945	3.94E-03

234.951	3.95E-03
235.418	1.32E-05
235.532	8.06E-03
239.292	1.00E-07
261.909	1.41E-08
263.397	3.75E-08
270.226	5.41E-02
271.048	2.36E-01
271.056	2.36E-01
277.794	1.85E-01
277.800	1.85E-01
282.055	2.83E-03
299.058	1.12E-02
299.061	1.09E-02
301.528	8.38E-05
301.868	2.56E-01
301.880	2.55E-01
314.144	3.06E-07
318.809	4.72E-04
322.175	1.18E-01
322.184	1.12E-01
322.197	9.11E-03
343.956	1.04E-01
347.283	3.79E-02
347.298	3.79E-02
370.513	3.58E-08
376.248	4.11E-04
376.578	6.25E-07
385.582	2.42E-05
386.623	8.96E-06
387.797	2.21E-01
387.815	2.21E-01
395.281	2.15E-03
404.574	7.40E-02
404.602	7.39E-02
416.677	1.44E-02
416.715	7.23E-03
416.721	6.71E-03
422.358	9.62E-08
439.878	1.95E-02
439.901	1.96E-02
447.417	2.04E-02
452.196	7.15E-07
468.158	1.88E-01
468.171	1.88E-01
483.064	2.61E-05
490.318	9.19E-05
491.778	8.06E-01
491.785	8.07E-01
495.524	1.70E+00

498.936	1.18E-05
504.016	3.47E-05
504.037	2.73E-05
512.879	1.17E-06
517.704	1.87E-01
526.667	3.84E+00
526.688	3.84E+00
538.339	5.43E-02
538.348	5.51E-02
554.705	1.19E-01
569.741	1.27E-05
577.550	5.55E-04
582.608	4.86E-05
585.696	5.37E+00
585.718	5.37E+00
592.220	1.93E-05
606.251	3.10E+00
612.418	7.62E+00
616.318	3.20E-02
616.322	3.19E-02
616.955	3.24E-06
633.061	3.21E-06
648.127	1.75E-03
648.156	1.76E-03
692.368	2.09E-04
692.410	2.24E-04
693.834	2.06E-06
695.042	7.53E-02
704.427	9.11E-01
726.725	4.84E+00
726.834	2.56E+00
726.854	2.56E+00
745.251	1.68E+00
745.286	1.69E+00
751.282	1.71E-05
773.067	2.40E+00
773.089	2.40E+00
807.759	3.32E-08

**(TiC)<sub>24</sub>**

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
116.064	2.32E-02
142.051	3.64E-06
159.793	4.53E-04
160.747	2.54E-02
165.516	2.76E-02
166.007	2.21E-02
171.451	7.00E-07

182.962	6.31E-08
183.100	3.75E-06
184.902	1.93E-06
185.816	6.78E-07
191.077	9.85E-07
194.749	1.84E-06
206.151	3.32E-06
217.208	2.92E-07
219.884	8.88E-03
230.308	1.92E-02
231.800	4.25E-06
234.218	3.05E-06
236.950	4.24E-04
237.697	1.09E-03
238.220	6.46E-02
238.568	4.02E-04
251.675	9.74E-06
251.737	2.36E-05
253.985	2.90E-02
255.492	1.51E-02
257.359	4.78E-02
259.577	2.26E-02
261.100	8.49E-06
270.871	1.91E-03
276.216	1.03E-04
278.911	1.58E-03
279.415	9.23E-02
281.074	4.73E-07
281.978	7.40E-06
285.199	6.49E-06
296.256	2.47E-05
299.890	5.19E-05
300.836	5.01E-01
302.623	2.24E-04
304.126	1.02E-02
305.163	3.69E-04
307.059	1.60E-01
308.516	6.60E-05
313.184	9.37E-06
331.664	4.54E-01
331.976	8.85E-02
334.756	2.55E-04
335.133	2.17E-03
341.898	3.42E-05
346.175	7.71E-05
352.999	4.98E-05
356.484	9.22E-03
360.809	3.33E-01
366.384	1.76E-01
377.981	4.73E-05

382.664	6.00E-02
383.800	7.63E-02
384.015	5.27E-04
385.883	7.88E-05
388.146	3.56E-03
391.636	6.30E-06
395.278	1.55E-04
395.507	1.51E-05
397.278	8.38E-06
406.263	5.19E-05
409.717	4.62E-02
420.795	6.72E-06
427.580	1.53E-02
427.789	2.02E-02
432.993	1.16E-05
434.992	1.41E-02
436.321	4.84E-02
438.817	3.54E-01
442.114	2.71E-05
445.853	7.78E-02
447.057	6.62E-06
448.435	1.60E-05
471.584	3.03E-05
474.309	1.83E-05
476.924	4.86E-06
479.288	6.49E-01
480.517	6.15E-05
484.650	3.21E-03
485.417	6.27E-05
489.153	2.43E-04
493.005	2.53E-04
496.887	8.24E-01
498.554	9.98E-01
504.134	7.72E-01
507.204	7.24E-05
507.768	6.52E-05
518.698	7.97E+00
523.535	2.32E-04
530.256	3.74E-01
546.119	1.33E-04
553.311	8.11E-05
556.575	2.85E+00
562.763	3.49E-01
574.254	2.20E-04
578.371	2.63E-04
583.935	1.33E+01
584.664	4.52E+00
584.994	2.31E-01
590.101	3.10E-03
590.332	7.48E+00

591.468	7.59E-02
602.218	4.02E-04
608.096	4.63E-04
610.646	2.76E+00
612.589	8.17E-04
612.784	2.51E-01
618.633	1.33E-04
624.599	2.80E-04
634.230	7.13E-04
640.858	3.03E-05
647.212	1.78E-04
671.589	2.98E+00
671.618	4.03E-01
675.304	5.34E-05
680.199	5.53E-02
694.368	3.00E-05
701.923	4.67E-05
704.423	1.70E-03
706.433	4.10E+00
709.321	9.28E-01
710.138	5.67E+00
719.757	9.63E-01
721.336	3.88E-04
731.879	9.86E-04
735.325	5.22E+00
735.684	4.23E+00
738.073	8.38E-05
738.422	1.73E-03
742.800	1.85E-03
783.762	6.68E-05
785.806	1.17E+00

**(TiC)<sub>32</sub>**

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
127.619	2.69E-07
127.742	2.13E-07
153.861	2.92E-06
154.053	1.45E-06
154.121	1.87E-06
157.087	5.74E-04
157.182	5.71E-04
157.289	7.52E-04
172.770	7.12E-02
172.898	7.15E-02
173.060	7.06E-02
179.663	1.62E-05
184.841	1.40E-05
185.080	4.15E-05



191.126	1.04E-02
191.275	1.07E-02
191.391	1.08E-02
206.590	1.17E-06
206.666	3.20E-06
206.761	1.61E-06
210.696	4.05E-06
210.744	4.30E-06
215.804	1.83E-06
230.719	1.20E-06
230.741	9.74E-07
230.776	2.18E-06
239.997	3.79E-05
240.018	3.10E-05
240.041	1.82E-05
240.645	7.67E-04
240.847	6.67E-04
240.980	5.01E-04
243.279	1.01E-04
249.486	1.93E-06
249.569	2.29E-06
249.621	3.17E-06
261.769	4.54E-05
261.794	4.92E-06
263.949	3.63E-02
264.072	3.60E-02
264.098	3.55E-02
270.586	5.25E-07
270.698	1.10E-05
270.860	2.10E-06
278.365	1.70E-03
278.400	1.66E-03
278.491	1.89E-03
286.916	5.41E-03
287.003	5.32E-03
287.065	5.60E-03
289.230	1.08E-05
289.293	3.99E-06
292.258	2.21E-06
302.907	5.71E-05
308.713	2.60E-06
308.763	9.74E-06
310.769	5.56E-06
310.822	3.22E-05
310.961	2.44E-05
315.904	5.08E-02
315.990	5.01E-02
316.060	4.95E-02
327.529	1.37E-01
327.593	1.39E-01

327.651	1.37E-01
334.319	5.30E-05
334.374	6.41E-05
334.436	4.43E-05
337.842	1.22E-04
344.125	8.92E-05
344.270	8.14E-05
356.957	9.18E-02
357.227	9.37E-02
357.509	9.32E-02
367.601	2.42E-02
367.715	2.67E-02
367.840	2.69E-02
381.125	1.07E-05
381.209	9.43E-06
381.292	7.05E-05
384.192	9.98E-06
385.443	5.35E-05
385.544	2.61E-05
385.654	1.41E-05
386.610	3.73E-05
386.717	2.61E-06
402.163	4.90E-05
404.525	1.71E-02
404.690	1.64E-02
404.711	1.66E-02
414.975	1.54E-01
415.103	1.54E-01
415.287	1.50E-01
424.091	5.35E-05
424.188	8.06E-06
424.214	4.89E-05
437.111	9.84E-05
437.145	1.45E-04
438.756	2.32E-02
439.078	1.02E-01
439.098	7.83E-02
439.117	1.01E-01
450.329	7.72E-05
450.488	2.76E-05
450.575	9.93E-05
458.446	7.80E-04
458.481	3.63E-04
459.747	5.13E-01
459.823	5.03E-01
459.865	4.96E-01
471.082	6.12E-02
471.121	6.80E-02
471.131	6.30E-02
474.111	2.54E-05

474.145	9.25E-05
474.189	1.43E-04
485.249	5.58E-05
485.303	5.02E-05
485.331	3.74E-05
494.769	8.53E-03
494.806	9.37E-04
495.754	1.78E+00
495.790	1.78E+00
495.932	1.76E+00
497.267	7.17E-03
533.805	7.72E-01
533.882	7.52E-01
533.936	7.51E-01
544.269	7.09E-04
544.370	4.71E-05
550.502	4.98E-04
566.699	9.31E+00
566.813	9.31E+00
566.900	9.37E+00
575.458	3.70E-04
575.528	7.28E-04
575.558	2.45E-04
579.832	1.70E-02
579.890	1.43E-02
581.562	6.10E+00
581.773	6.23E+00
581.838	6.21E+00
598.896	1.47E-03
599.381	7.14E-04
608.023	4.69E-04
608.030	6.48E-05
608.157	4.85E-05
609.457	9.13E-01
609.491	9.24E-01
609.500	9.28E-01
615.785	8.03E-05
615.826	4.03E-05
615.853	9.13E-05
628.600	3.19E-04
628.630	4.48E-04
628.659	2.87E-04
628.767	4.59E-04
628.900	8.90E-04
652.882	3.78E-05
652.912	2.67E-06
652.964	3.03E-05
679.270	8.01E-01
679.328	8.02E-01
679.401	7.74E-01

694.266	7.02E-03
694.294	3.47E-03
699.135	6.87E+00
699.358	6.78E+00
699.458	6.82E+00
703.627	9.35E-03
709.308	6.41E-04
709.329	1.61E-03
711.315	1.17E-01
711.353	2.38E-01
711.378	3.34E-01
711.415	6.79E-01
711.518	1.32E+00
711.612	1.29E+00
714.111	3.47E-04
721.906	4.70E-04
721.919	5.92E-04
721.966	1.51E-03
751.836	6.06E-01
752.024	6.42E-01
752.128	6.29E-01
760.037	1.29E-04

**(TiC)<sub>40</sub>**

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
101.732	2.24E-06
122.880	2.58E-03
126.001	3.92E-03
133.221	2.44E-02
138.274	5.22E-05
140.614	4.73E-06
156.749	2.11E-05
159.165	1.42E-04
162.447	1.03E-04
165.138	3.83E-02
166.984	5.21E-02
168.602	3.93E-05
169.378	1.99E-04
180.286	2.02E-05
181.159	1.05E-01
183.350	2.01E-04
183.742	4.07E-06
187.104	8.52E-06
197.091	1.85E-05
198.512	7.60E-03
199.853	6.62E-05
204.524	2.14E-06
206.520	2.78E-03

207.032	1.21E-02
208.793	1.98E-06
210.503	2.19E-06
214.535	1.19E-04
217.071	9.16E-03
218.199	3.41E-05
219.584	2.64E-03
226.434	6.63E-06
229.576	2.28E-04
232.706	1.11E-02
235.409	3.28E-05
237.373	2.55E-03
237.904	1.57E-03
238.751	1.70E-05
244.383	8.95E-07
248.153	9.74E-07
248.233	3.16E-06
248.993	7.41E-04
252.269	7.14E-07
257.004	4.75E-06
258.729	5.11E-05
259.039	3.78E-04
260.627	8.10E-06
260.837	2.48E-05
262.709	2.48E-04
265.833	2.64E-06
266.388	1.79E-01
268.560	4.69E-06
270.061	2.21E-05
271.938	5.90E-02
273.277	2.15E-03
273.825	5.12E-05
274.439	1.85E-05
276.355	1.07E-05
277.980	6.15E-07
281.413	5.34E-05
281.670	7.89E-04
282.247	1.37E-06
287.788	8.31E-07
288.458	4.53E-05
291.576	1.51E-05
291.756	3.54E-03
296.313	2.17E-02
297.935	2.47E-05
299.139	4.25E-03
299.667	4.05E-05
300.833	5.19E-03
305.049	8.34E-05
305.680	1.40E-01
306.590	2.09E-03

308.504	4.03E-01
313.885	3.82E-02
314.350	5.07E-05
314.734	4.34E-05
319.457	1.47E-03
320.504	1.51E-04
323.329	1.21E-01
326.934	8.76E-05
331.149	7.30E-05
334.465	2.30E-01
336.443	4.45E-01
337.373	1.14E-02
338.874	1.06E-04
339.926	2.72E-04
340.924	5.14E-05
345.496	4.40E-04
349.010	3.06E-04
350.350	1.36E-01
350.913	5.60E-02
352.686	7.29E-02
362.476	5.66E-05
366.341	2.85E-06
368.907	2.81E-05
370.775	3.45E-05
371.610	1.52E-03
376.617	4.25E-02
377.286	1.48E-04
381.122	5.48E-05
381.666	6.41E-05
382.645	5.35E-03
387.325	1.34E-05
387.639	2.36E-06
389.939	3.25E-05
391.406	6.38E-03
391.919	5.39E-05
394.842	9.69E-06
395.731	9.31E-04
396.340	1.90E-01
401.458	9.36E-02
402.416	9.63E-04
406.949	7.34E-02
413.326	6.74E-05
414.913	1.68E-01
421.309	2.69E-01
422.371	1.99E-04
423.809	6.39E-03
424.980	3.04E-05
427.079	3.63E-05
427.288	1.10E-05
429.686	6.36E-05

432.338	2.83E-02
433.446	2.99E-04
437.009	3.45E-03
437.406	1.20E-04
438.327	5.91E-02
443.904	1.78E-05
448.151	7.20E-02
449.853	1.17E-03
450.346	4.17E-05
450.977	1.55E-04
453.379	3.51E-04
453.979	1.97E-02
454.509	5.40E-05
455.733	5.81E-01
459.234	2.77E-01
465.826	4.14E-01
468.238	5.52E-05
470.528	8.62E-05
473.653	4.89E-03
474.000	2.50E-01
474.927	1.10E-02
478.504	1.97E-04
482.339	3.69E-04
485.416	2.07E-04
487.945	1.05E+00
488.528	1.40E+00
488.634	9.21E-03
488.876	3.71E-02
491.534	6.64E-05
492.842	1.62E+00
492.983	1.12E-02
496.561	9.98E-05
522.069	1.81E+00
522.507	1.36E+00
529.248	2.03E-03
534.611	3.85E+00
534.845	3.10E+00
535.377	2.71E-02
539.659	8.19E-04
543.814	1.34E-03
545.190	5.88E-04
552.251	8.84E+00
558.410	1.09E+00
564.871	1.03E+01
564.957	1.11E-01
566.657	1.33E+01
567.823	3.03E-04
569.993	2.50E-03
573.976	1.20E-03
575.740	2.15E-01

576.081	1.90E-02
579.029	9.18E+00
583.926	7.25E-04
591.881	2.59E-04
593.047	1.13E-03
593.308	2.68E-04
595.101	2.70E-01
595.526	1.50E-02
596.156	2.42E+00
601.953	2.38E-04
604.355	3.82E-04
605.214	4.72E-05
607.250	1.25E+00
608.284	5.50E-03
608.416	4.66E-03
612.553	1.22E-04
615.208	1.02E-01
621.340	9.86E-03
624.549	5.92E-02
624.674	4.47E-01
625.277	4.61E-04
625.549	4.68E-03
627.295	5.02E-05
628.541	3.09E-02
632.006	1.69E-05
643.214	5.37E-05
646.250	1.28E-05
649.636	7.44E-05
655.622	1.17E+00
667.698	6.55E-03
668.931	6.77E-01
676.105	3.87E-05
679.747	1.05E+01
686.447	6.52E-01
686.482	2.15E+00
688.195	5.04E+00
690.694	1.02E-03
691.991	1.04E-02
693.743	5.01E+00
694.848	8.38E-05
695.914	3.60E-04
700.473	1.80E+00
703.090	2.65E-01
703.972	2.98E-03
704.599	1.79E-04
706.647	4.20E-04
707.217	1.33E-03
708.348	3.15E-01
708.627	2.13E+00
709.029	3.31E-03



713.246	1.07E-03
717.094	8.79E-05
718.591	2.74E-05
718.757	5.91E-04
721.249	6.18E-01
721.381	1.70E-01
722.817	3.21E-01
745.639	2.72E-04
748.859	1.26E+00
758.348	1.29E+00
762.104	8.47E-05

(TiC)<sub>50</sub>

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
93.018	1.10E-06
119.502	7.22E-06
121.455	1.47E-05
124.209	1.75E-05
131.442	3.46E-03
131.853	3.17E-03
133.536	8.34E-03
138.769	2.58E-03
139.697	2.97E-03
151.851	4.33E-05
154.980	3.01E-04
155.490	2.38E-04
156.969	1.81E-04
164.083	1.19E-02
171.443	4.29E-02
171.904	4.31E-02
181.168	2.63E-05
184.969	2.43E-05
186.353	9.98E-04
187.574	3.16E-02
187.872	3.10E-02
190.781	2.17E-04
191.448	2.07E-03
191.704	2.28E-03
196.347	6.24E-06
198.546	1.55E-05
200.957	1.56E-05
202.891	5.12E-05
203.135	7.11E-06
210.552	5.57E-06
213.612	3.42E-03
214.136	9.60E-03
214.391	5.84E-03
216.561	6.53E-03

216.703	7.24E-03
216.915	2.84E-03
222.760	6.91E-03
229.920	1.79E-05
230.230	2.12E-06
231.476	3.04E-05
231.785	7.88E-05
234.562	1.73E-05
237.670	3.95E-05
242.049	1.62E-03
242.174	1.53E-03
245.974	1.96E-03
246.426	1.52E-02
246.604	1.68E-02
247.102	2.14E-04
247.380	2.91E-04
251.582	3.03E-03
255.698	1.32E-05
256.645	4.79E-04
256.717	5.90E-04
256.812	7.12E-04
260.873	2.96E-03
260.952	9.10E-03
262.318	1.85E-02
262.431	2.01E-02
263.498	1.25E-02
263.671	1.03E-02
266.546	3.89E-05
268.511	2.73E-03
268.938	1.35E-01
269.057	1.32E-01
269.570	1.33E-02
272.881	5.60E-03
272.962	5.59E-03
275.099	2.10E-05
275.526	3.60E-05
277.445	3.51E-05
277.944	3.65E-02
279.914	1.69E-02
279.975	1.73E-02
286.016	2.40E-04
287.417	8.13E-03
287.558	1.98E-02
287.954	6.44E-02
288.217	7.83E-02
288.616	9.11E-04
293.029	1.08E-03
293.536	9.22E-05
294.620	1.26E-01
294.714	1.29E-01

295.308	9.31E-03
295.595	5.64E-02
295.703	5.14E-02
296.004	9.73E-04
300.670	4.51E-03
303.801	2.49E-05
306.348	1.03E-02
306.714	1.61E-02
310.942	2.56E-01
311.122	2.17E-01
311.304	3.47E-02
314.209	1.42E-05
315.276	7.10E-05
315.842	1.11E-02
315.947	1.51E-02
320.863	1.16E-04
325.304	3.63E-04
325.841	2.22E-01
327.011	3.20E-01
327.202	3.30E-01
329.997	1.05E-04
333.611	2.91E-02
336.572	1.20E-01
336.892	1.03E-01
339.111	1.74E-02
339.315	1.71E-02
346.078	2.98E-02
346.261	5.35E-02
346.378	5.26E-02
349.340	1.36E-05
352.227	2.00E-04
352.518	2.61E-05
355.936	9.67E-05
359.989	3.79E-05
364.619	1.86E-02
364.699	1.44E-02
365.020	9.54E-02
368.265	3.42E-05
369.268	9.81E-04
373.870	2.82E-02
374.030	8.64E-03
374.204	1.69E-02
374.300	4.61E-02
374.794	1.78E-04
375.815	8.07E-03
380.264	7.60E-03
381.179	3.52E-02
381.472	3.74E-02
386.744	5.22E-03
387.007	5.58E-03

387.265	2.20E-04
395.825	2.28E-04
396.988	1.07E-05
400.633	1.72E-01
400.773	1.88E-01
401.900	6.28E-02
402.009	6.75E-02
402.617	2.17E-03
405.220	3.11E-04
405.905	5.26E-02
409.775	3.39E-02
409.935	1.72E-02
410.561	2.79E-01
413.741	6.44E-05
415.982	1.08E-03
418.419	1.54E-04
422.756	2.93E-02
422.760	2.82E-02
423.595	2.05E-04
426.388	2.43E-05
426.535	6.12E-05
426.947	3.42E-06
429.330	8.99E-05
429.762	4.22E-05
432.624	2.04E-04
432.898	5.59E-03
432.978	6.89E-03
436.242	4.15E-02
436.727	1.01E-01
436.807	1.01E-01
438.433	1.25E-04
446.246	3.25E-04
446.677	6.83E-04
449.487	8.19E-02
449.666	9.65E-02
451.443	2.74E-01
451.472	2.58E-01
455.536	1.62E-01
456.276	1.30E-04
456.602	1.33E-04
462.036	4.26E-03
462.216	5.90E-03
465.833	3.79E-02
466.037	3.80E-02
467.597	7.49E-02
470.752	1.58E-04
477.610	1.32E-02
477.652	1.63E-02
483.642	4.65E-04
484.948	2.71E-01

485.208	2.60E-01
486.337	2.40E-03
486.646	1.34E-04
486.853	1.30E-03
487.039	1.67E-02
489.908	6.79E-01
490.297	6.25E-01
495.476	1.88E+00
518.611	1.09E-02
520.465	1.12E+00
520.645	8.20E-01
521.221	5.97E-02
523.376	5.33E+00
523.400	5.44E+00
527.746	2.58E+00
529.043	2.93E-03
532.645	3.84E+00
532.661	3.98E+00
533.644	3.12E-01
541.564	3.33E-03
545.550	1.61E-03
547.230	2.19E+00
548.218	2.20E+00
548.529	2.17E+00
550.866	2.44E-03
554.813	2.91E+00
554.998	2.78E+00
562.250	2.74E+00
562.425	1.95E+00
562.722	8.97E+00
564.147	6.68E-03
568.101	2.45E-03
577.229	1.70E-01
577.348	1.40E-01
580.381	6.98E-04
581.424	1.43E+00
585.831	7.69E-01
585.864	8.42E-01
586.620	2.33E+00
590.562	8.98E-04
591.655	6.21E-03
592.399	1.69E-03
594.046	1.24E+00
594.051	1.27E+00
598.641	8.50E-04
601.854	2.85E-02
603.796	1.41E-01
603.862	1.42E-01
605.560	4.70E-04
608.239	3.96E-04

608.562	7.41E-02
608.713	6.85E-02
619.399	8.20E-02
619.654	7.97E-02
620.100	5.33E-04
620.646	2.16E-03
621.935	4.62E-02
622.040	5.45E-02
623.491	3.33E-04
624.199	4.08E-01
624.366	4.09E-01
626.220	2.07E-04
627.281	7.55E-05
630.607	5.51E-05
638.358	9.19E-01
638.419	8.91E-01
641.871	3.16E-01
641.910	3.08E-01
656.227	6.43E-04
659.777	3.97E-01
662.148	2.28E+00
662.872	2.16E+00
669.886	1.94E-04
670.473	6.43E-02
671.577	3.66E+00
671.755	3.96E+00
673.573	2.83E+00
676.706	4.04E-03
684.837	5.72E-01
684.903	5.79E-01
688.791	9.86E-01
688.809	9.25E-01
689.254	1.05E-01
689.468	5.33E-01
691.385	3.18E-02
691.549	1.01E-01
693.644	4.14E-03
693.822	1.07E-02
697.460	2.05E-03
699.087	1.00E+00
702.016	1.69E+00
702.126	1.51E+00
704.421	1.08E+00
704.583	1.31E+00
704.764	1.81E-02
709.008	3.65E-04
709.129	2.38E-04
712.835	5.66E-04
713.340	5.93E-01
713.450	3.30E-01

713.753	7.14E-01
716.481	1.47E+00
716.665	2.85E-02
723.665	3.04E-03
725.413	1.25E-02
725.531	1.19E-02
737.416	3.65E-04
752.311	1.12E+00
752.556	1.15E+00
764.575	5.72E-01

### Ti<sub>18</sub>C<sub>14</sub>

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
132.418	3.04E-06
137.663	4.84E-06
147.137	4.31E-03
147.672	4.12E-03
163.957	2.32E-05
179.697	1.07E-03
182.489	5.33E-04
188.870	2.64E-04
191.903	1.47E-02
194.008	2.44E-02
205.184	2.58E-04
211.495	2.82E-01
212.085	2.66E-01
213.990	9.56E-02
222.979	7.07E-02
226.581	1.48E-03
228.079	9.38E-03
228.435	9.34E-03
230.897	2.59E-05
239.497	4.86E-05
243.980	1.87E-03
244.334	2.98E-03
247.858	2.82E-05
257.874	4.72E-07
263.860	7.26E-06
271.193	4.25E-05
271.969	1.12E-05
275.020	3.15E-04
275.819	3.52E-04
289.220	4.51E-02
300.741	8.29E-05
302.628	7.93E-03
302.799	9.91E-03
303.445	2.89E-02
303.751	3.10E-02

314.218	4.35E-02
320.806	6.77E-02
341.853	7.17E-02
349.355	2.07E-02
349.652	1.90E-02
351.944	3.26E-05
362.423	1.69E-01
362.589	1.72E-01
374.530	8.12E-02
381.914	1.42E-02
386.063	9.37E-05
387.587	1.51E-04
399.071	2.38E-02
399.284	2.40E-02
423.167	7.43E-04
425.686	8.27E-02
425.840	8.44E-02
426.823	5.00E-01
449.707	4.52E-02
449.798	4.53E-02
451.862	3.35E-04
458.083	2.67E-04
461.644	2.85E-02
493.630	5.41E-01
493.784	5.51E-01
499.941	1.51E+00
503.905	2.75E-01
504.273	2.38E-01
508.300	6.82E-04
518.306	2.15E-03
523.449	3.46E+00
523.879	3.50E+00
542.795	1.15E+00
560.760	5.01E-05
574.219	1.18E+00
604.665	1.19E+00
605.311	1.22E+00
613.716	1.59E-02
622.750	5.19E-05
644.080	3.11E-02
645.477	2.88E-02
647.141	4.04E-03
665.569	2.03E+00
675.716	5.54E-01
676.702	5.77E-01
686.546	3.27E+00
697.553	2.89E-02
698.154	2.16E-02
707.426	1.37E-04
712.039	1.15E-01



712.727	1.16E-01
727.904	6.80E-01
747.909	2.54E+00
747.971	2.57E+00
790.237	3.66E-05

**Ti<sub>17</sub>C<sub>18</sub>**

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
54.080	3.41E-01
88.263	2.47E-02
131.843	3.12E-01
139.494	1.48E-02
142.377	4.30E-02
150.851	6.29E-04
157.214	3.71E-02
170.887	6.55E-03
174.920	6.14E-03
176.624	2.85E-02
178.441	4.73E-02
187.272	1.78E-01
191.831	6.65E-02
193.708	9.21E-02
201.223	2.97E-02
208.001	1.19E-02
210.473	7.16E-02
214.292	2.99E-02
225.715	1.36E-01
232.371	2.83E-02
239.930	4.70E-02
240.815	8.76E-02
242.042	8.14E-02
247.068	4.42E-04
250.404	1.19E-01
252.115	9.84E-02
262.896	8.51E-02
270.407	4.69E-01
276.011	4.76E-02
279.333	5.24E-01
280.114	6.59E-02
285.982	1.54E-01
290.698	1.67E-01
296.040	7.68E-02
300.214	1.02E-01
307.184	1.13E-01
316.204	1.01E-01
323.971	1.88E-01
331.546	6.89E-03
345.948	1.38E-01

359.684	1.14E-01
362.844	2.57E-01
366.042	1.64E-01
373.665	9.32E-01
383.660	2.27E-04
391.762	6.04E-02
406.745	2.01E-01
415.862	3.53E-01
443.632	1.63E-01
457.985	4.07E-01
459.230	4.57E-02
471.447	2.30E-05
474.056	2.56E-02
481.850	2.90E-01
486.372	1.33E-02
490.281	5.45E-03
491.752	3.84E-01
493.707	1.48E-01
494.942	3.14E-01
502.287	4.12E-01
505.662	1.02E+00
507.102	4.02E-01
507.817	2.80E-01
511.823	9.05E-01
514.432	3.66E-01
520.196	2.19E-04
522.687	9.63E-03
524.986	8.65E-02
530.251	5.84E-01
531.356	3.92E-02
532.769	2.78E-01
536.978	5.28E-01
541.389	8.74E-01
548.189	1.56E+00
553.268	2.27E-01
555.153	1.29E-01
561.166	7.71E-01
572.577	1.36E+00
573.293	4.73E+00
574.824	4.47E+00
583.839	1.11E-01
584.683	2.43E-02
587.577	2.62E+00
595.235	5.59E-01
607.760	5.87E-01
608.654	3.86E-02
621.145	5.23E-02
628.963	3.13E-02
640.744	1.93E+00
644.605	6.07E-01

644.779	6.39E-01
654.407	9.53E-01
654.913	3.70E-02
677.284	6.06E-01
682.364	4.87E-01
683.549	1.22E-03
690.031	4.95E-02
698.660	9.26E-01
731.595	2.22E-01

### Ti<sub>24</sub>C<sub>20</sub>

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
120.300	2.51E-03
130.758	4.22E-06
150.710	8.50E-03
160.087	1.80E-05
163.692	6.62E-03
166.561	2.24E-02
169.946	7.14E-07
171.926	5.62E-06
177.658	2.21E-05
181.542	1.03E-05
185.602	2.71E-06
189.486	8.54E-05
192.727	1.12E-05
197.118	2.86E-04
198.028	8.52E-04
201.348	1.63E-03
203.668	6.26E-01
207.338	3.37E-05
212.055	4.92E-02
213.875	1.37E-01
216.374	1.95E-06
223.010	1.40E-04
224.470	1.33E-02
229.130	6.15E-05
231.036	5.05E-02
238.187	9.35E-02
238.239	2.23E-02
239.396	3.11E-05
244.935	4.86E-02
245.180	1.70E-03
247.415	7.21E-02
248.442	6.24E-04
249.061	3.14E-02
257.546	1.07E-02
257.930	1.55E-04
260.735	1.57E-02

268.263	2.10E-03
271.234	2.26E-02
278.670	1.65E-06
283.023	2.57E-05
291.601	1.73E-06
294.356	1.12E-05
298.730	2.79E-06
300.079	2.58E-05
302.288	1.40E-02
305.706	2.62E-06
306.071	6.43E-06
306.810	1.23E-06
308.801	3.27E-03
314.669	3.29E-04
328.599	8.59E-06
328.995	1.95E-06
342.003	2.40E-02
349.614	1.68E-02
349.847	4.51E-02
350.791	2.95E-01
356.421	1.87E-02
363.584	8.04E-06
368.833	1.24E-06
371.309	2.96E-06
375.031	3.17E-04
375.340	7.84E-03
381.141	2.11E-05
390.531	4.30E-02
397.186	1.56E-04
397.953	3.52E-02
406.504	1.30E-01
412.093	3.17E-06
438.719	2.90E-06
451.844	2.77E-05
460.429	6.35E-06
464.060	1.06E-04
465.557	4.98E-04
468.685	1.80E-01
470.209	5.80E-02
480.035	1.79E-05
497.408	1.50E-04
500.687	4.52E-01
501.035	1.14E-02
501.447	1.20E+00
505.712	1.52E-04
508.442	6.05E-04
510.099	4.03E-01
513.280	6.51E-02
518.450	4.62E-05
520.041	7.42E-05

526.945	9.56E-05
534.321	9.61E-01
534.529	1.01E-03
538.111	2.33E-01
547.172	5.46E+00
547.424	1.60E-03
553.935	2.38E-04
556.176	4.65E+00
559.729	7.92E-05
563.592	6.18E-04
565.667	2.49E+00
565.988	2.19E-02
575.882	6.04E-05
584.723	5.85E-01
600.083	4.00E-05
600.233	9.20E-05
608.137	3.05E-03
609.514	8.69E-05
624.686	1.54E-01
629.328	4.47E+00
631.273	1.24E-02
640.222	5.73E-03
641.144	7.25E-01
648.387	7.47E-04
648.922	1.55E-04
651.585	8.50E-01
657.070	2.92E-04
658.726	5.56E-04
664.590	1.46E-05
670.017	4.01E-05
672.957	1.19E-05
678.969	1.87E-01
682.262	2.47E-05
687.067	8.71E-02
687.139	1.70E-02
688.425	5.44E-03
696.463	4.40E+00
703.056	1.51E-05
760.895	2.40E+00
761.833	2.02E-04

### Ti<sub>23</sub>C<sub>24</sub>

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
11.124	1.91E-04
12.499	1.52E-03
98.728	2.99E-01
123.257	1.97E-01
127.504	1.33E-01

152.464	6.38E-02
154.900	4.31E-02
167.293	1.74E-02
172.823	1.07E-01
175.231	1.92E-04
180.495	8.76E-02
185.384	1.53E-02
188.858	2.16E-02
193.232	2.91E-02
199.809	3.90E-02
204.153	3.66E-01
207.679	7.78E-03
210.730	4.85E-02
217.578	9.88E-03
225.648	1.67E-02
229.037	1.63E-03
237.355	9.86E-03
239.204	8.47E-04
239.803	1.38E-02
251.846	4.04E-02
253.487	3.75E-02
254.483	7.68E-02
254.655	1.20E-02
258.295	2.73E-01
258.732	3.27E-03
261.446	6.38E-02
265.203	3.26E-02
271.984	3.23E-03
275.841	9.54E-03
278.031	9.72E-02
280.540	2.15E-01
282.636	2.15E-02
283.618	3.02E-02
288.369	1.06E-01
289.571	2.10E-02
297.949	9.64E-02
300.471	2.29E-02
302.237	4.58E-02
305.328	6.71E-02
307.078	3.01E-01
311.283	1.20E-01
314.834	5.61E-02
315.067	6.32E-02
325.707	8.61E-02
328.609	3.41E-01
333.268	1.33E-03
338.054	8.26E-02
338.384	2.22E-01
346.962	1.14E-01
352.232	4.05E-03

357.880	5.38E-01
365.826	1.57E-01
367.796	1.17E-01
370.945	1.20E-01
381.008	8.12E-03
382.526	2.23E-01
384.114	7.07E-02
387.810	2.63E-02
392.114	1.44E-04
392.874	4.37E-04
396.816	7.77E-03
402.790	6.00E-02
403.030	6.56E-02
406.595	1.04E-01
418.698	3.98E-03
420.592	5.11E-02
423.711	6.65E-03
426.135	4.34E-03
436.683	4.20E-02
438.705	5.06E-02
440.746	1.72E-02
445.556	4.61E-02
446.018	3.54E-01
453.989	1.69E-03
454.524	7.25E-03
465.051	4.94E-01
473.353	3.62E-01
476.299	1.23E+00
476.939	1.88E-01
480.067	1.42E-02
482.075	5.03E-01
483.599	7.70E-03
485.472	4.76E-01
493.523	3.39E-01
494.153	8.21E-01
496.147	8.55E-01
496.347	3.77E-01
498.184	5.92E-04
500.560	8.22E-01
511.328	2.84E-01
517.971	8.45E-02
527.646	3.59E+00
538.059	9.80E-03
547.149	2.10E+00
548.233	6.58E-01
567.828	3.74E+00
568.236	8.32E-01
570.176	1.42E+00
574.156	6.31E+00
581.407	3.01E+00

581.880	1.83E+00
586.037	3.78E+00
587.793	9.14E-02
599.258	2.63E-01
604.195	1.57E+00
611.928	3.61E-03
619.492	4.69E-03
620.587	4.85E-03
632.084	1.16E-02
642.025	1.11E-02
646.967	2.40E-02
660.744	7.09E-02
666.122	3.51E+00
668.128	1.55E-03
672.898	2.83E-02
680.136	7.54E-01
682.332	3.78E-01
692.438	1.19E+00
693.163	3.86E-01
693.513	9.06E-01
701.249	3.41E-01
704.799	3.19E-02
717.270	5.16E-01
721.119	8.54E-02
722.588	4.78E-02
729.130	1.53E+00
729.567	4.75E-01
735.304	2.34E+00
738.651	2.58E-02
781.702	7.17E-01

### Ti<sub>32</sub>C<sub>28</sub>

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
118.549	1.08E-05
118.724	4.36E-06
150.544	4.73E-05
150.702	8.36E-05
150.918	8.52E-05
155.832	2.40E-04
156.696	5.20E-04
157.218	1.61E-03
167.719	1.60E-01
168.198	1.56E-01
168.491	1.55E-01
179.945	1.75E-05
180.723	3.28E-04
186.358	3.04E-04
186.936	1.07E-03



187.586	2.86E-05
191.315	7.09E-02
191.353	7.47E-02
191.617	7.62E-02
208.105	4.86E-05
208.156	5.01E-04
208.224	5.07E-04
214.359	6.28E-04
215.516	9.54E-04
215.789	1.35E-03
222.610	1.72E-01
222.788	3.92E-02
222.820	1.03E-02
223.174	1.77E+00
223.608	1.91E+00
224.038	1.88E+00
230.316	3.00E-03
230.428	4.56E-03
230.511	8.65E-05
238.973	2.20E-03
244.018	1.51E-01
244.225	1.56E-01
244.327	1.58E-01
248.750	3.18E-02
248.943	2.99E-02
249.072	2.77E-02
251.975	1.82E-04
252.095	1.74E-04
252.146	9.23E-05
255.783	9.41E-05
261.321	6.01E-03
261.393	6.58E-03
261.554	5.40E-03
262.433	3.23E-04
262.513	3.52E-05
280.315	3.05E-01
280.422	3.17E-01
280.500	3.15E-01
288.062	1.02E-05
288.120	5.66E-05
288.410	4.28E-05
296.910	6.20E-05
300.776	6.09E-05
300.905	2.15E-04
304.471	2.15E-04
313.410	4.29E-04
313.535	1.18E-03
313.627	3.11E-04
314.537	3.39E-02
314.570	3.35E-02

314.799	3.32E-02
320.116	1.62E-04
320.368	2.20E-04
330.445	5.91E-04
330.503	7.11E-04
330.547	3.96E-04
336.561	2.92E-01
336.766	3.03E-01
337.070	3.07E-01
361.515	3.59E-02
361.702	3.27E-02
361.880	3.54E-02
366.633	1.04E-04
366.718	3.13E-04
366.802	2.56E-04
368.472	3.14E-04
369.067	4.53E-04
374.062	2.83E-01
374.196	2.81E-01
374.245	2.86E-01
380.403	6.93E-05
380.436	4.44E-04
380.886	1.66E-04
394.785	1.28E-01
395.173	1.21E-01
395.427	1.28E-01
411.365	2.02E-04
411.564	6.56E-04
411.772	5.29E-04
412.060	6.50E-05
436.490	1.67E-03
444.416	1.95E+00
444.605	1.98E+00
444.990	1.98E+00
462.381	2.22E-03
462.802	6.92E-03
462.961	3.32E-03
471.901	2.58E+00
472.026	2.49E+00
472.384	2.55E+00
482.269	4.68E-03
482.497	7.60E-03
495.280	6.47E-01
495.415	6.85E-01
495.583	6.41E-01
497.369	1.09E-02
503.727	6.70E-04
503.864	2.23E-04
504.102	3.60E-04
512.033	1.19E-01

512.461	1.24E-01
512.503	1.25E-01
515.204	2.57E-03
515.376	4.29E-05
523.402	2.81E-04
523.693	2.38E-05
523.917	3.77E-04
551.069	2.44E-02
553.703	2.09E+00
553.835	1.95E+00
553.960	1.80E+00
554.256	2.69E-01
554.554	1.32E-02
554.607	1.89E-01
555.700	2.95E-01
555.880	2.15E-02
556.922	2.67E+00
557.022	3.22E+00
557.486	3.39E+00
596.027	9.30E-06
596.608	3.91E-04
596.928	1.75E-04
597.134	3.72E-04
610.488	7.69E-02
610.726	1.66E-01
610.877	2.48E-01
611.147	3.52E-01
611.173	3.97E-01
611.449	3.97E-01
622.550	5.33E-05
622.714	2.70E-04
635.445	1.76E-01
635.557	1.71E-01
635.760	1.76E-01
639.582	9.55E-06
639.674	7.73E-04
639.704	3.46E-04
651.109	2.07E+00
651.169	2.12E+00
651.305	2.13E+00
663.283	7.69E-04
663.462	9.99E-05
665.374	2.77E-04
665.424	4.48E-04
667.091	4.51E-04
675.083	7.77E-04
675.210	4.01E-04
675.292	1.78E-03
675.659	2.56E-02
675.807	2.64E-02

675.899	2.21E-02
684.998	5.33E-01
685.172	5.35E-01
685.326	5.30E-01
698.665	2.01E-04
714.841	8.74E-03
715.888	2.28E+00
716.257	2.35E+00
716.413	2.34E+00

### Ti<sub>31</sub>C<sub>32</sub>

Frequency (cm <sup>-1</sup> )	Intensity (arb. units)
66.510	5.10E-01
67.496	5.06E-01
114.593	4.21E-01
135.919	3.87E-02
136.441	3.96E-02
155.507	3.70E-05
159.214	3.17E-02
159.748	2.10E-03
160.399	9.42E-03
163.153	1.35E-01
163.649	1.30E-01
172.671	1.94E-01
177.716	9.63E-02
178.027	9.40E-02
180.613	1.15E-04
185.409	1.02E-02
185.635	7.80E-03
190.094	7.05E-02
200.881	5.05E-02
200.947	5.15E-02
206.150	1.20E-06
209.444	2.00E-02
209.584	2.09E-02
221.851	1.09E-02
227.702	5.00E-03
227.710	4.94E-03
230.133	1.65E-05
237.965	3.07E-02
238.150	3.01E-02
239.750	2.68E-03
241.711	1.07E-02
241.873	1.40E-02
242.383	7.29E-06
244.768	1.48E-01
244.806	1.46E-01
246.422	2.21E-04

248.320	1.28E-02
257.851	3.60E-02
257.996	3.59E-02
263.814	1.89E-03
263.853	1.72E-03
268.398	2.33E-02
268.456	2.34E-02
272.454	2.97E-05
272.514	6.97E-05
275.292	1.25E-02
275.486	2.07E-03
282.584	2.84E-02
282.858	2.28E-02
283.009	2.47E-02
287.120	4.35E-03
287.203	4.04E-03
290.627	4.34E-02
291.387	7.51E-02
291.436	7.57E-02
293.127	1.41E-05
307.651	1.11E-02
307.781	1.57E-02
307.918	8.31E-03
312.004	4.54E-02
312.130	4.52E-02
312.519	1.89E-04
316.713	4.32E-02
323.056	8.89E-02
323.137	9.11E-02
328.753	2.51E-02
328.896	2.66E-02
330.350	3.56E-01
335.296	2.05E-02
340.721	2.31E-05
344.101	4.13E-02
344.256	4.10E-02
354.783	4.91E-02
355.480	5.34E-02
359.008	3.30E-02
365.508	2.03E-02
365.664	1.86E-02
375.835	1.49E-02
376.070	4.44E-03
376.083	4.06E-03
378.405	5.84E-05
383.381	3.20E-03
383.408	2.68E-03
384.813	2.50E-05
385.760	5.84E-03
385.922	5.36E-03

401.792	6.55E-03
401.932	6.19E-03
402.572	8.39E-03
410.044	1.25E-01
410.680	8.39E-02
410.874	8.55E-02
415.845	3.84E-02
415.918	3.94E-02
417.323	7.59E-05
425.973	2.44E-05
426.054	8.14E-05
431.935	2.43E-05
435.170	2.79E-03
439.177	1.19E-01
440.270	4.99E-02
440.340	3.77E-02
440.789	1.91E-01
440.979	1.96E-01
458.177	4.47E-03
458.392	2.97E-01
458.505	3.00E-01
458.601	2.88E-01
462.658	1.43E-01
462.671	1.33E-01
467.309	2.93E-01
470.474	8.52E-04
470.549	2.92E-04
474.459	9.64E-02
474.583	8.95E-02
479.119	1.14E-04
481.939	3.39E-03
482.142	4.76E-03
488.162	3.98E-03
489.714	9.22E-04
491.959	9.95E-01
492.034	9.83E-01
492.728	2.60E-01
492.847	3.44E-01
497.772	1.73E+00
512.652	6.56E-02
512.748	6.96E-02
517.689	1.06E+00
536.349	6.08E-01
536.403	5.93E-01
544.902	1.83E-01
556.439	3.78E+00
559.696	8.34E+00
559.866	8.36E+00
568.318	1.30E-03
573.330	4.61E+00

573.744	4.76E+00
576.031	1.93E-01
576.276	2.86E-01
576.365	6.56E+00
590.353	6.76E-01
590.403	7.13E-01
590.960	3.50E-02
598.193	3.30E-04
604.109	4.79E-04
606.889	9.64E-01
610.829	2.39E-03
610.873	2.53E-03
613.831	7.73E-05
616.458	6.73E-02
616.490	6.04E-02
626.416	1.88E-03
626.476	1.09E-03
628.021	4.46E-03
628.139	5.35E-03
629.785	2.23E-02
648.946	1.10E-01
649.034	1.13E-01
652.074	2.26E-05
667.382	1.07E-01
667.565	1.06E-01
675.815	2.54E-02
677.816	1.87E+00
677.899	1.87E+00
682.589	2.80E+00
691.665	1.63E+00
691.669	1.63E+00
699.504	7.10E-01
699.682	7.40E-01
700.408	3.54E-01
707.136	1.36E+00
707.162	1.37E+00
708.771	3.28E-03
708.800	4.53E-03
709.804	4.16E-02
711.284	2.32E-04
711.932	5.82E-01
716.303	6.16E-01
716.416	6.48E-01
717.973	4.93E-01
750.049	6.67E-01
750.095	6.80E-01
755.688	2.97E-01