## THE JOURNAL OF PHYSICAL CHEMISTRY J. Phys. Chem. B, 1998, 102(44), 8923-8929, DOI:10.1021/jp982316n

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		excitation wavelength/nm							
$\Delta v/cm^{-1}$		530.9	566	568.2	588	601	612	647.1	<u>676.4</u>
212	1.24	0.33/0.31	1.19/1.05	0.77/1.14	1.01/1.72	2.16/1.97	1.87/2.03	1.09/1.03	0.60/0.60
251	0.69	0.19/0.14	0.47/0.47	0.53/0.51	0.88/0.76	0.87/0.87	0.88/0.90	0.64/0.44	0.26/0.26
274	1.18	0.66/0.49	1.90/1.63	1.65/1.78	2.40/2.63	3.01/3.00	3.06/3.09	1.81/1.49	0.95/0.87
326	0.43	/0.09	0.32/0.31	0.42/0.34	0.42/0.49	0.65/0.56	0.47/0.57	0.25/0.27	0.18/0.15
346	0.93	0.14/0.51	1.67/1.65	1.56/1.80	2.19/2.62	3.26/2.95	2.61/3.02	1.61/1.39	0.89/0.80
360	0.60	0.26/0.23	0.83/0.74	0.87/0.80	1.25/1.16	1.09/1.31	1.39/1.33	0.91/0.61	0.45/0.35
375	1.27	1.17/1.12	3.47/3.63	4.24/3.93	5.74/5.71	6.12/6.40	6.69/6.51	4.02/2.95	2.16/1.68
399	1.30	1.55/1.36	3.89/4.38	5.01/4.75	6.74/6.86	7.18/7.67	7.83/7.77	4.56/4.47	2.98/1.97
412	1.28	1.87/1.42	4.30/4.56	5.78/4.94	7.33/7.11	7.76/7.93	8.04/8.03	4.45/3.56	2.60/2.01
428	1.08	1.29/1.11	3.07/3.55	4.30/3.85	5.64/5.52	5.94/6.14	6.30/6.20	3.66/2.72	2.26/1.53
443	0.43	0.19/0.19	0.48/0.59	0.76/0.64	1.01/0.92	0.74/1.02	1.05/1.02	0.62/0.45	0.36/0.25
460	0.58	0.40/0.37	1.03/1.18	1.46/1.28	1.93/1.82	1.75/2.02	2.05/2.03	1.29/0.87	0.72/0.49
654	0.22	0.18/0.12	0.55/0.37	0.24/0.40	0.30/0.54	0.53/0.58	0.58/0.57	0.34/0.22	0.19/0.12

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## Table 3. Absolute Resonance Raman Cross Sections of A. denitrificans Azurin

The resonance Raman cross sections are shown as experimental/calculated in units of Å<sup>2</sup>/molecule /10<sup>-10</sup>. A --- indicates no cross section was measured. The errors in cross sections are ±10% for strong lines and ±20% for weak lines. The  $\Delta$ 's are in dimensionless normal coordinates. The cross-sections were calculated with Equation 1 using the following parameters: zero-zero energy, E<sub>0</sub> = 14,300 cm<sup>-1</sup>, transition length, M = 0.73 Å, temperature, T = 0 K, refractive index, n = 1.33, Lorentzian homogeneous linewidth,  $\Gamma_L = 450$  cm<sup>-1</sup>, Gaussian homogeneous linewidth,  $\Gamma_G = 75$  cm<sup>-1</sup> inhomogeneous linewidth,  $\Theta = 150$  cm<sup>-1</sup>.

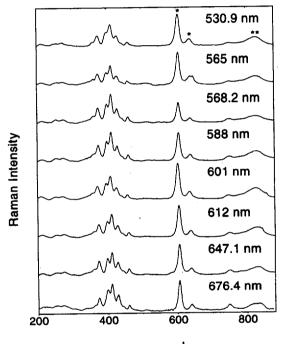
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## **Figure Legend**

Figure 8: Resonance Raman spectra of *A. denitrificans* azurin at excitation wavelengths throughout the absorption band. The spectra are the sum of three to five scans. The vibrations between 200 and 500 cm<sup>-1</sup>, and the peak at 654 cm<sup>-1</sup> were used in the analysis. Raman scattering of the internal intensity standard (cacodylate) is observed at 608 and 638 cm<sup>-1</sup> (\*). The broad band at ~820 cm<sup>-1</sup> and the narrower band at ~755 cm<sup>-1</sup> (\*\*) are composed of the overtones and combinations of the azurin vibrations between 350 and 500 cm<sup>-1</sup> and a cacodylate peak at 825 cm<sup>-1</sup>.

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Energy (cm<sup>-1</sup>)