

### Electronic Supporting Information

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**Table S1.** The IR absorption maxima for isolated CD<sub>3</sub>CN in solid noble gas matrices, cm<sup>-1</sup>.

CD <sub>3</sub> CN				
Type of mode	Ne	Ar	Kr	Xe
ν <sub>1</sub> (CH str.)	2128.6	2122.1 (2122.1*)	2116.2	2115.7
	2123.6	2118.2 (2118.3*)	2114.2	2111.8
ν <sub>2</sub> (CN str.)	2275.6		2264.7	2270
	2273.6	2267.1 (2267.3*)	2259.5	2267.2
ν <sub>3</sub> (CH <sub>3</sub> def.)	1109.6	1104.4 (1104.7*)	1102.9	1104.1
	1107.5	(1103.3*)	1098.4	1101.2
ν <sub>4</sub> (CC str.)	836	831.1 (831.1*)	832.9	835.7
	833	829.0 (829.7*)	830.8	831.5
		(829.1*)	827.7	829.5
ν <sub>5</sub> (CH str.)		2253.7 (2253.7*)	2247	2249.8
ν <sub>6</sub> (CH <sub>3</sub> def.)	1050.1	1045.5 (1046.8*)	1043.6	1042.1
	1048	1042.7 (1043.1*)	1040.5	1038
	1046.1	1040.1 (1040.1*)	1037.9	1034.5
	1041.6	1036.9 (1036.9*)	1032.6	1029.4
ν <sub>7</sub> (CH <sub>3</sub> rock)	851.7	(852.5*)	848.3	848
	848	849.3 (849.5*)	844.5	845
		845.6 (845.5*)	838.3	841.8
ν <sub>7</sub> + ν <sub>8</sub>	1195	1187.9 (1189.7*)	1188.5	1185.7
	1192.6	1183.3 (1183.7*)	1181.4	1182.5
	1184.7	(1182.9*)	1174.3	1180.8

\*Taken from: T. B. Freedman and E. R. Nixon, *Spectrochim. Acta Part A Mol. Spectrosc.*, 1972, **28** by (Freedman and Nixon 1972)