

Inorganic Chemistry

including bioinorganic chemistry

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Table S1. Analytical Compositions and ^{205}Ti NMR Parameters for the Studied Solutions. (The chemical shifts δ_m , signal integrals I_m and spin-spin coupling constants J_m ($^1J_{^{205}\text{Ti}-^{13}\text{C}}$), refer to the exchange-averaged NMR signal for the species with composition $\text{Ti}(\text{CN})_m\text{Cl}_n$. Integrals in *italics* were not used in the final calculations.

a.) Extracted from NMR Spectra Recorded on MSL90 spectrometer (for some solutions, spectra were also recorded on AM400 as indicated in the leftmost column)

m	I_4	J_1	J_2	J_3	J_4													
M	mM	kHz	kHz	kHz	kHz													
400	2.0094	0.05019	0	0	2090.97					50.19								
400	0.0503	0.05053	0	0.3002	2540.18					50.53								
400	0.6997	0.05026	0.09982	0.1008	2259.26	2418.16	2491.29			40.71	8.20	1.35						
	0.3766	0.05022	0.1590	0.0910	2282.84	2449.53	2525.10			29.26	14.26	6.70						
	0.1772	0.05024	0.1693	0.1114	2379.97	2570.61	2660.13			26.61	15.37	8.28						
	0.4429	0.05018	0.1793	0.0605	2243.33	2398.39	2471.18			17.27	18.44	14.47						
	0.6987	0.05018	0.1499	0.05083	2216.11	2363.86	2436.19			15.08	18.13	16.97						
	1.3556	0.05018	0.08002	0.02010	2200.29	2337.99	2413.75			6.82	11.98	31.38						
	0.0502	0.05037	0.0998	0.2003	2536.58	2752.55	2855.89	2946.89		17.95	15.88	14.17	2.37					
	0.1135	0.05025	0.1699	0.1205	2488.05	2689.18	2788.19	2915.78		13.98	16.54	17.18	2.55					
400	0.0501	0.05030	0.1491	0.1510	2533.46	2752.15	2856.01	2946.99	3005.10	2.55	8.34	24.53	13.38	1.50		9.094	6.958	
400	0.0500	0.05021	0.2006	0.09950		2749.52	2855.29	2946.87	3005.27		0.19	8.04	24.10	17.89			7.019	
400	0.0499	0.05006	0.3000	0					3007.13					50.06				
400	0.05009	0.05030	0.1491	0.1510												9.094	6.958	
400	0.05001	0.05021	0.2006	0.09950													7.019	5.432
	1.994	0.04845	0.05101	0	2089.72	2312.82	2414.60			12.42	15.08	20.95						
	1.519	0.04952	0.06562	0.03376	2201.20	2339.88	2415.15			14.27	14.05	21.19						
	1.364	0.04987	0.07042	0.04484	2201.25	2342.96	2416.69			17.13	16.31	16.43						
	1.046	0.05058	0.08019	0.06742	2208.88	2353.97	2425.98			26.74	15.70	8.14						

b.) Extracted from NMR Spectra Recorded on AM400 spectrometer

[illegible]

Figure S1. Predominance diagram for the $\text{Ti}(\text{CN})_m\text{Cl}_n^{3-m-n}$ complexes in acidic aqueous solution containing 3 M $\{(\text{H}^+ + \text{Li}^+), \text{ClO}_4^-\}$ as ionic medium. 25 °C. $[\text{Ti}(\text{III})]_{\text{tot}} = 0.050 \text{ M}$.

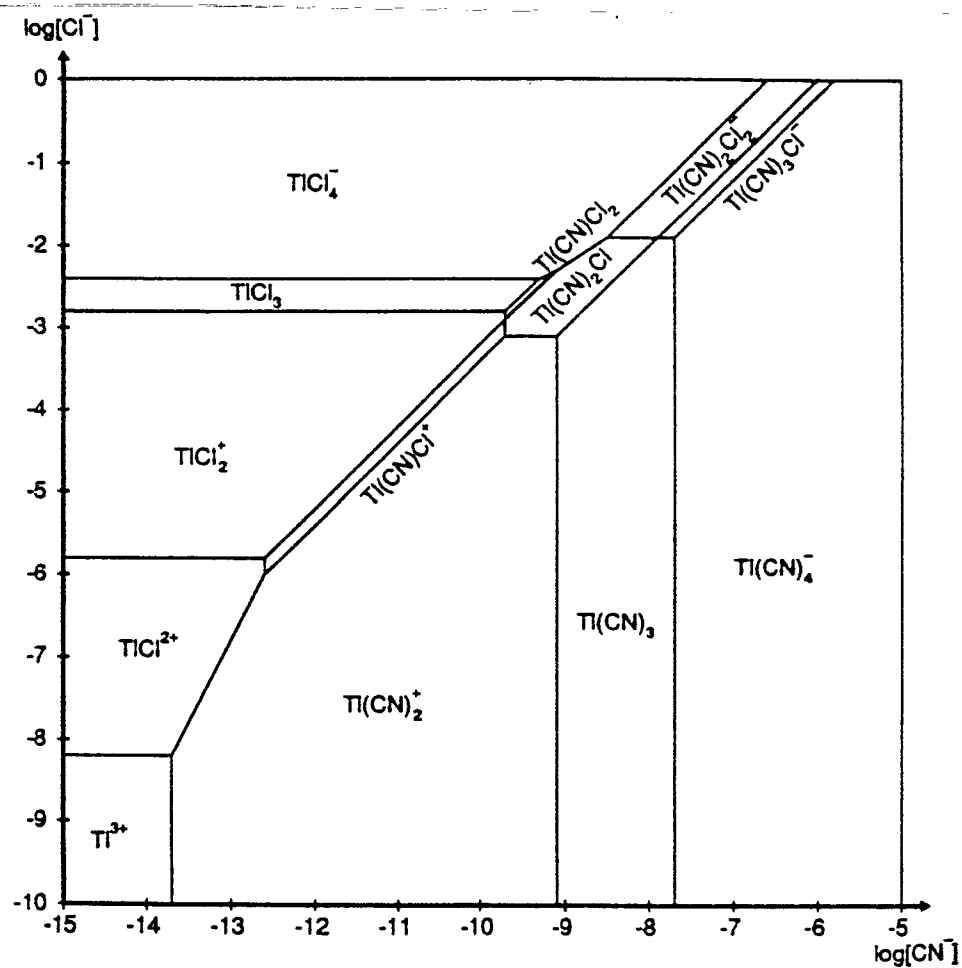


Figure S2. Correlation between the spin-spin coupling constants, $^1J(^{205}\text{Ti}-^{13}\text{C})$, for the complexes $\text{Ti}(\text{CN})_m\text{Cl}_n^{3-m-n}$ ($m+n \leq 4$) and the Ti-CN force constant.²⁰

