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When the Inhibitor Tells More than the Substrate: the Cyanide-Bound State of a Carbon Monoxide Dehydrogenase

Alexandre Ciaccafava,[a†*] Daria Tombolelli,[a†] Lilith Domnik,[b] Jochen Fesseler,[b] Jae-Hun Jeoung,[b] Holger Dobbek,[b] Maria Andrea Mroginski,[a*] Ingo Zebger,[a*] Peter Hildebrandt[a]

Table S1. Statistics on Data collection and structure refinement.

	–320 mV CN^- - soaked
Data collection	
X-ray source	Beamline 14.1, BESSY II
Wavelength (Å)	0.91841
Space group	*C*2
Cell dimensions	
a, *b*, *c* (Å)	112.2, 75.5, 71.2
α, β, γ (°)	90.0, 111.5, 90.0
Total / unique reflections	594,333 / 159,430
R_{meas} (%) [a]	6.2 (61.7)
Resolution (Å)	40.764 – 1.23 (1.235 – 1.229)
Completeness (%)	99.4 (98.5)
$I / \sigma I$	14.55 (2.44)
Refinement	
R_{work} / R_{free} (%) [b]	11.77 / 14.67
protein molecules in the ASU	1
Ramachandran – statistics (%)	
preferred / allowed / disallowed	96.3 / 3.2 / 0.5
Rms deviation from ideal geometry	
Bond lengths (Å)	0.015
Bond angles (°)	1.567
ESU [c]	0.023

Values in parentheses are for highest-resolution shell.
[a] Redundancy independent R-factor (intensities)[1]
[b] The R_{free} factor was calculated from 5% of the data, which were removed at random before the refinement was carried out.
[c] Estimated overall coordinate error (ESU) based on maximum likelihood.

Reference

1 Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275

[a] *Technische Universität Berlin, Institut für Chemie, Sekretariat PC 14, D–10623 Berlin, Germany. E-mails: alex.ciacca@gmail.com, andrea.mroginski@tu-berlin.de, ingo.zebger@tu-berlin.de*
[b] *Humboldt-Universität zu Berlin, Institut für Biologie, Unter den Linden 6, D–10099 Berlin, Germany.*
† These authors contributed equally.

Table S2. Accuracy of the QM method

	Wavenumber / cm^{-1}		
Sample	ν(CN)exp.	ν(CN)calc.	Δν (CNexp. - CNcalc.)
$[Fe(CN)_6]^{4-}$	2037	2024	13
$[Ni(CN)_4]^{2-}$	2124	2118	6

Calculated vibrational frequency of cyanide stretching on two model compounds and comparison with experimentally assigned peaks in solution. QM: DFT with BP86/def2-TZVP/6-31g* with RI. Optimization was performed with Turbomole, frequencies were calculated with Gaussian09.