

C(CN)₅⁻ : transition state or intermediate?

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Table S1. Cartesian coordinates (in Å), total energies (in kcal/mol),^a number of imaginary frequencies and imaginary frequencies if any (in cm⁻¹) of stationary points computed at OLYP/TZ2P.

C(CN)₄: T_d symmetry
-1626.1972 kcal/mol
no imaginary frequencies

C	0.000032	0.000043	1.382681
C	0.000000	0.000000	-0.103008
C	-1.400732	-0.000031	-0.598207
C	0.700365	-1.213066	-0.598217
C	0.700336	1.213054	-0.598288
N	-2.493208	-0.000055	-0.984429
N	1.246601	-2.159176	-0.984447
N	1.246550	2.159154	-0.984573
N	0.000057	0.000077	2.541418

CN⁻: C_{∞v} symmetry
-371.0419 kcal/mol
no imaginary frequencies

C	0.000000	0.000000	2.338427
N	0.000000	0.000000	3.522794

TS: C(CN)₅⁻: D_{3h} symmetry
-2004.0028 kcal/mol
IMAGINARY FREQUENCY (A₂'') : -471.223

C	0.000000	0.000000	2.119898
N	0.000000	0.000000	3.291530
C	0.000000	0.000000	0.000000
C	1.445099	0.000000	0.000000
C	-0.722550	1.251493	0.000000
C	-0.722550	-1.251493	0.000000
C	0.000000	0.000000	-2.119898
N	0.000000	0.000000	-3.291530
N	2.606026	0.000000	0.000000
N	-1.303013	2.256885	0.000000
N	-1.303013	-2.256885	0.000000

NCCN: C_{∞h} symmetry
-725.4295 kcal/mol
no imaginary frequencies

N	0.000000	0.000000	1.852615
C	0.000000	0.000000	0.687330
C	0.000000	0.000000	-0.687330
N	0.000000	0.000000	-1.852615

C(CN)₃⁻: D_{3h} symmetry
-1353.3194 kcal/mol
no imaginary frequencies

C	-0.702374	-1.220765	0.000000
C	1.408397	0.002108	0.000000
C	-0.706028	1.218653	0.000000
N	-1.287651	-2.238012	0.000000
N	2.581997	0.003866	0.000000
N	-1.294350	2.234141	0.000000
C	-0.000002	-0.000002	0.000000

Complex [NCCN, C(CN)₃⁻]: C_s symmetry
-2082.2018 kcal/mol
no imaginary frequencies

C	-0.702830	1.220626	0.001815
C	-0.702830	-1.220626	0.001815
N	-1.289884	2.235920	0.003023
N	-1.289884	-2.235920	0.003023
C	0.001371	0.000000	-0.000003
C	4.604897	0.687684	-2.460321
C	4.604897	-0.687684	-2.460321
C	1.406184	0.000000	-0.000544
N	4.691023	-1.847117	-2.545801
N	4.691023	1.847117	-2.545801
N	2.580395	0.000000	0.004445

^a Evaluated relative to ADF's basic atoms.