Electronic supplementary materials *Mendeleev Commun.*, 2022, **32**, 457–459

Decomposition of dinitrosyl iron complex with thioformaldehyde ligands in water: reaction mechanisms and the role of chemical hardness of ligands

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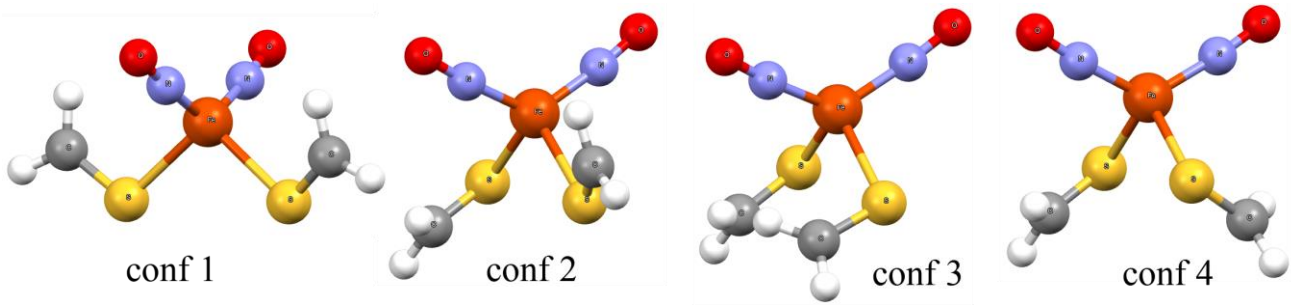

Figure S1 The optimized structure of the conformations of DNIC **1**.

Table S1 Electronic energies $E_{el,w}$, zero-point vibrational energies *ZPVE*, thermal free-energy corrections at 298K $G_{298,w}$, relative free energies ΔG_w for the conformations of **1** (see Figure S1) from the M06/def2TZVP calculations in water.

Conformation	$E_{el,w}$, a.u.	*ZPVE* , a.u.	$G_{298,w}$, a.u.	ΔG_w kJ mol^{-1}
1	–2398.296819	0.067027	0.023299	0.0
2	–2398.297646	0.067498	0.024766	1.7
3	–2398.298615	0.068331	0.026101	2.6
4	–2398.297953	0.068005	0.026649	5.8

Table S2 Coordinates of the optimized structures of selected reactants in Figure 1 (see main text).

Species **1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.066393	0.048434	0.177018
2	7	0	-1.326634	1.034274	0.897880
3	7	0	1.093655	-0.968399	1.008661
4	8	0	-2.128217	1.633718	1.466338
5	8	0	1.811331	-1.620611	1.629901
6	16	0	1.183315	1.427225	-1.405368
7	16	0	-1.218571	-1.454947	-1.367585
8	6	0	2.321618	2.082553	-0.470443
9	6	0	-1.895319	-2.520558	-0.365632
10	1	0	-1.789030	-2.471645	0.715743
11	1	0	-2.493502	-3.335324	-0.768801
12	1	0	2.411481	1.873430	0.592907
13	1	0	3.040245	2.776583	-0.901493

Species **2**

1	26	0	0.085034	-0.067215	-0.115831
2	7	0	-0.832663	1.065200	0.895078
3	7	0	1.001528	-1.212922	0.881328
4	8	0	-1.274367	1.613585	1.817490
5	8	0	1.435192	-1.801760	1.782253
6	16	0	-1.886521	-1.757202	-0.406741
7	16	0	2.167441	1.589680	-0.277460
8	6	0	-2.296853	-2.069255	1.116604
9	6	0	2.515822	1.770344	1.281919
10	1	0	-1.797220	-1.612604	1.971413

11	1	0	-3.105662	-2.761342	1.343735
12	1	0	1.956430	1.278675	2.078067
13	1	0	3.341620	2.405477	1.597526
14	8	0	0.006472	-0.066957	-2.222560
15	1	0	-0.225879	0.782400	-2.617404
16	1	0	0.806809	-0.360746	-2.674131

Species **TS1**

1	26	0	0.104101	-0.110966	-0.347289
2	7	0	-0.656761	1.122986	0.674676
3	7	0	1.060943	-1.263160	0.603037
4	8	0	-1.083794	1.705961	1.582066
5	8	0	1.507864	-1.834952	1.508779
6	16	0	-2.019288	-1.559106	-0.366034
7	16	0	2.601968	1.667865	0.056104
8	6	0	-2.267868	-1.805808	1.204467
9	6	0	2.522104	1.677807	1.659920
10	1	0	-1.614241	-1.413202	1.982913
11	1	0	-3.121750	-2.390679	1.540705
12	1	0	1.760252	1.138053	2.224225
13	1	0	3.240403	2.235943	2.259342
14	8	0	0.152686	0.005107	-2.408936
15	1	0	0.301944	-0.821804	-2.882640
16	1	0	-0.591376	0.441319	-2.840047

Species **3**

1	26	0	0.517389	-0.171762	0.424734
2	7	0	1.514506	-0.990598	-0.789813
3	7	0	0.677715	1.596141	0.425103
4	8	0	2.085958	-1.235268	-1.768948
5	8	0	0.833186	2.687078	0.063743
6	8	0	-0.256007	-1.113203	2.083724
7	16	0	-1.548986	-0.192619	-0.974516
8	6	0	-1.072523	0.624207	-2.277977
9	1	0	-0.069799	1.033316	-2.395856
10	1	0	-1.766680	0.792849	-3.098613
11	1	0	0.209780	-1.912306	2.356574
12	1	0	-0.312544	-0.547688	2.863145

Species **TS2**

1	26	0	-0.592300	-0.721854	0.784269
2	7	0	-1.196878	0.836828	1.412157
3	7	0	1.112152	-0.638158	0.262096
4	8	0	-1.291471	1.965773	1.679632

5	8	0	2.162290	-0.247272	-0.049917
6	16	0	-0.920755	0.876431	-1.901875
7	6	0	0.015259	2.115134	-1.491466
8	1	0	0.500820	2.198151	-0.518016
9	1	0	0.205750	2.939000	-2.178679
10	8	0	-1.856704	-2.113248	-0.159056
11	1	0	-1.495432	-2.468782	-0.980143
12	1	0	-2.724922	-1.758376	-0.385270
13	8	0	-0.431490	-1.902922	2.547724
14	1	0	-0.040677	-2.756821	2.324119
15	1	0	-1.315018	-2.106765	2.878933

Species **4**

1	26	0	0.037423	-0.219325	-0.020157
2	7	0	-1.562985	0.587173	-0.050017
3	7	0	1.373637	0.966814	-0.068541
4	8	0	-2.364068	1.431806	-0.078081
5	8	0	2.048204	1.913404	-0.091942
6	8	0	0.152421	-1.754869	-1.439632
7	8	0	0.222986	-1.389326	1.697358
8	1	0	-0.617670	-1.765658	-2.021046
9	1	0	0.917509	-1.668318	-2.020640
10	1	0	0.956452	-1.121275	2.263546
11	1	0	-0.564856	-1.353376	2.253511

Species **TS3**

1	26	0	0.276347	0.816518	0.559998
2	7	0	-1.064732	1.710663	-0.172526
3	7	0	0.014600	-0.449373	1.774029
4	8	0	-2.072270	2.034908	-0.638647
5	8	0	-0.397366	-1.323091	2.410282
6	16	0	1.983732	0.084047	-1.086237
7	16	0	-1.057128	-1.428232	-1.177933
8	6	0	3.094209	-0.655008	-0.179453
9	6	0	-2.450243	-1.416308	-0.378078
10	1	0	-2.671505	-0.715894	0.428430
11	1	0	-3.244414	-2.123825	-0.614470
12	1	0	3.061314	-0.669315	0.907249
13	1	0	3.924808	-1.172514	-0.655342

Species **5**

1	26	0	-0.725009	0.069233	-0.809084
2	7	0	-0.775597	1.533297	0.199973

3	7	0	-1.015868	-1.404680	0.143394
4	8	0	-0.672412	2.201957	1.141572
5	8	0	-1.025641	-2.116721	1.058416
6	16	0	1.812220	-0.143405	-0.542074
7	6	0	1.947069	-0.185346	1.061823
8	1	0	1.100086	-0.129229	1.744659
9	1	0	2.929456	-0.274550	1.521164

Species **7**

1	26	0	-0.010051	0.333226	-0.404341
2	7	0	-1.514608	-0.550044	-0.047407
3	7	0	1.444353	-0.643999	-0.052117
4	8	0	-2.268661	-1.349352	0.330239
5	8	0	2.152874	-1.493701	0.301264
6	8	0	0.152955	2.232413	0.414083
7	1	0	-0.545278	2.427283	1.050972
8	1	0	0.984720	2.358000	0.886844