Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information for

Nanosecond time-resolved IR study of thiobenzoylnitrene

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Table S1. Thiobenzoylnitrene singlet **^{1}1** B3LYP/6-31G* optimized geometry (coordinates in Å) and energy.

Energy with zero point correction (Hartrees): -722.628403

Cartesian Coordinates:

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	3.616594	1.052406	0.000000
14	3.201528	-0.872064	0.000000
6	0.068296	-1.247380	0.000000
6	-1.270869	1.213398	0.000000
6	0.791943	-0.042220	0.000000
6	-1.321652	-1.211575	0.000000
6	-1.991154	0.016889	0.000000
6	0.121968	1.187557	0.000000
6	2.241622	-0.077352	0.000000
1	0.601484	-2.193331	0.000000
1	-1.885930	-2.139499	0.000000
1	-3.077444	0.039553	0.000000
1	0.697373	2.108482	0.000000
1	-1.793758	2.165137	0.000000

Table S2. Thiobenzoylnitrene triplet ^{3}**1** B3LYP/6-31G* optimized geometry (coordinates in Å) and energy.

Energy with zero point correction (Hartrees): -722.602479

Cartesian Coordinates:

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	3.428123	1.183646	0.000000
14	2.955828	-1.286764	0.000000
6	0.065959	-1.231648	0.000000
6	-1.201926	1.255266	0.000000
6	0.833743	-0.054083	0.000000
6	-1.323613	-1.160683	0.000000
6	-1.960919	0.082890	0.000000
6	0.190065	1.190028	0.000000
6	2.314233	-0.169631	0.000000
1	0.567451	-2.194714	0.000000
1	-1.910273	-2.074957	0.000000
1	-3.046147	0.137653	0.000000
1	0.782218	2.099668	0.000000
1	-1.694741	2.223329	0.000000

Table S3. Sulfoximine **12** B3LYP/6-31G* optimized geometry (coordinates in Å) and energy.

Energy with zero point correction (Hartrees): -1275.846264

Cartesian Coordinates:

Atomic Number	Coordinates (Angstroms) X	Y	Z
32	0.331029	2.462369	-0.688627
32	2.439630	0.046293	-0.545039
14	0.886680	-0.167200	-0.241666
8	2.942572	0.338522	-1.900463
6	-1.703735	-1.000707	-0.056900
6	-3.795173	0.835960	0.081767
6	-1.421816	0.373221	-0.165754
6	-3.011723	-1.447368	0.113459
6	-4.062835	-0.531291	0.183676
6	-2.489514	1.284020	-0.091906
6	-0.019306	0.850855	-0.363708
6	3.240774	1.176617	0.637796
6	3.058057	-1.563309	-0.023781
1	-0.887645	-1.710678	-0.117625
1	-3.211397	-2.513096	0.187939
1	-5.083839	-0.880055	0.315417
1	-2.276503	2.344042	-0.174847
1	-4.607075	1.556041	0.136898
1	4.319884	1.043652	0.528766
1	2.905825	0.935736	1.649204
1	2.935856	2.183458	0.357089
1	2.574208	-2.301416	-0.666064
1	2.796503	-1.741631	1.020434
1	4.139544	-1.574034	-0.176062

Table S4. B3LYP/6-31G* calculated frequencies (cm^{-1}, scaled by 0.96) and intensities for singlet thiobenzoylnitrene ^{1}**1**.

Frequency	Intensity	Frequency	Intensity
58	0.5	978	1.2
124	1.3	1012	1.6
128	1.2	1071	3.9
285	2.0	1150	0.1
372	1.0	1158	20.2
396	0.1	1180	19.7
453	2.1	1294	4.2
494	6.7	1316	5.1
540	13.4	1436	17.5
604	1.3	1476	3.0
670	27.1	1572	5.1
671	23.9	1592	8.9
746	32.8	1752	54.9
825	0.0	3066	0.1
833	40.2	3076	4.1
907	1.9	3082	9.2
938	0.0	3089	11.8
969	0.0	3093	10.2

Table S5. B3LYP/6-31G* calculated frequencies (cm^{-1}, scaled by 0.96) and intensities for triplet thiobenzoylnitrene ^{3}**1**.

Frequency	Intensity	Frequency	Intensity
36	0.6	977	1.9
142	0.4	1014	2.1
171	0.0	1072	5.1
294	1.6	1144	24.7
380	9.7	1149	0.7
394	0.0	1168	2.2
399	0.3	1292	4.2
468	3.9	1313	15.2
566	13.3	1380	220.9
605	0.5	1439	10.7
659	5.3	1477	0.4
675	26.6	1572	2.1
753	27.3	1590	5.0
823	9.2	3062	0.0
828	0.0	3072	9.7
911	2.3	3080	12.8
940	0.0	3087	10.5
966	0.1	3091	10.8

Table S6. B3LYP/6-31G* calculated frequencies (cm^{-1}, scaled by 0.96) and intensities for sulfoximine **12**.

Frequency	Intensity	Frequency	Intensity
17	1.1	945	0.6
37	2.6	966	1.6
89	2.9	972	82.6
102	2.5	976	10.6
154	0.5	981	19.0
166	0.3	1010	139.5
186	0.2	1019	1.8
193	0.1	1070	26.6
232	7.4	1145	0.2
255	0.7	1159	113.9
274	2.9	1169	198.8
324	1.1	1199	120.3
370	3.3	1251	505.9
373	27.2	1292	19.4
397	0.1	1303	118.1
414	33.5	1313	2.8
449	9.9	1329	42.6
597	14.3	1406	15.9
606	4.7	1419	0.1
615	0.4	1421	5.7
632	11.9	1436	18.7
668	21.5	1438	42.3
674	34.8	1473	0.8
706	19.8	1571	0.7
765	17.1	1591	10.5
828	0.5	2961	2.8
833	61.6	2965	1.4
916	1.9	3056	0.4
923	18.6	3057	0.7
927	10.0	3063	2.8

Table S7. B3LYP/6-31G* calculated charges and spins for triplet thiobenzoylnitrene ^{3}**1**.

Atom Number	Charge (a. u.)	Spin (a. u.)
1	0.163208	0.001887
1	0.143969	-0.000597
1	0.142815	0.001525
1	0.164159	0.000350
1	0.143380	-0.000683
6	-0.164212	-0.026676
6	-0.133043	0.027865
6	0.152323	0.079951
6	-0.129132	0.019241
6	-0.118369	-0.034485
6	-0.177034	-0.038697
6	0.023382	-0.279449
16	0.050022	0.958961
7	-0.261468	1.290806

Sum of atom charges = 0.000000
Sum of spin charges = 2.000000

Table S8. B3LYP/6-31G* calculated charges and spins for triplet thioacetylnitrene.

Atom Number	Charge (a. u.)	Spin (a. u.)
1	0.186924	0.005166
1	0.193329	-0.008769
1	0.193329	-0.008769
6	-0.477715	0.059923
6	0.075257	-0.289693
16	0.055094	0.971441
7	-0.226216	1.270702

Sum of atom charges = 0.000000
Sum of spin charges = 2.000000

Table S9. B3LYP/6-31G* calculated charges and spins for triplet thioformylnitrene.

Atom Number	Charge (a. u.)	Spin (a. u.)
1	0.207266	0.071191
6	-0.112504	-0.307305
16	0.077957	0.966161
7	-0.172719	1.269954

Sum of atom charges = 0.000000
Sum of spin charges = 2.000000

Table S10. B3LYP/6-31G* calculated charges and spins for triplet acetylnitrene.

Atom Number	Charge (a. u.)	Spin (a. u.)
1	0.191432	-0.005463
1	0.193135	0.008289
1	0.190353	-0.005133
6	-0.526886	0.025118
6	0.502009	-0.196271
8	-0.362868	0.423430
7	-0.187176	1.750030

Sum of atom charges = 0.000000
Sum of spin charges = 2.000000

Table S11. B3LYP/6-31G* calculated charges and spins for triplet formylnitrene.

Atom Number	Charge (a. u.)	Spin (a. u.)
1	0.151107	0.032763
6	0.304181	-0.218520
8	-0.309806	0.458603
7	-0.145482	1.727154

Sum of atom charges = 0.000000
Sum of spin charges = 2.000000