Supporting Information

for

Visible Mechanochromic Responses of Spiropyrans in Crystal *via* Pressure-Induced Isomerization

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1. Experimental Section

High pressure experiments were performed using symmetric diamond anvil cells (DACs) at room temperature. The culet diameter of the diamond anvils was 500 μm. The crystal was placed in the holes (diameter: ca. 170 μm) of a T301 steel gasket, which was pre-indented to a thickness of 50 μm. The silicon oil was used as pressure transmitting medium (PTM). A small ruby chip was inserted into the sample compartment for *in situ* pressure calibration according to the R1 ruby fluorescence method. High-pressure absorption spectra were recorded by an optical fiber spectrometer (Ocean Optics, QE65000). The optical images were obtained by using a Nikon Ti-U microscope equipped with a digital color camera. **SP-NO$_2$**, **SP-H**, **SP-Ph** were purchased from TCI company in >98% purity.

2. *In situ* UV-Vis Spectra

1) *In situ* UV-Vis Spectra for **SP-NO$_2$**

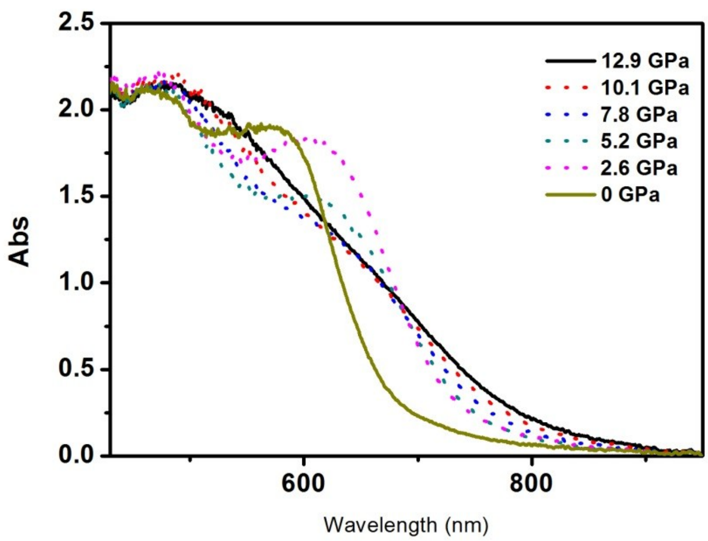

Figure S1. *In situ* UV-Vis spectroscopy of **SP-NO$_2$** under high pressure during decompression process.

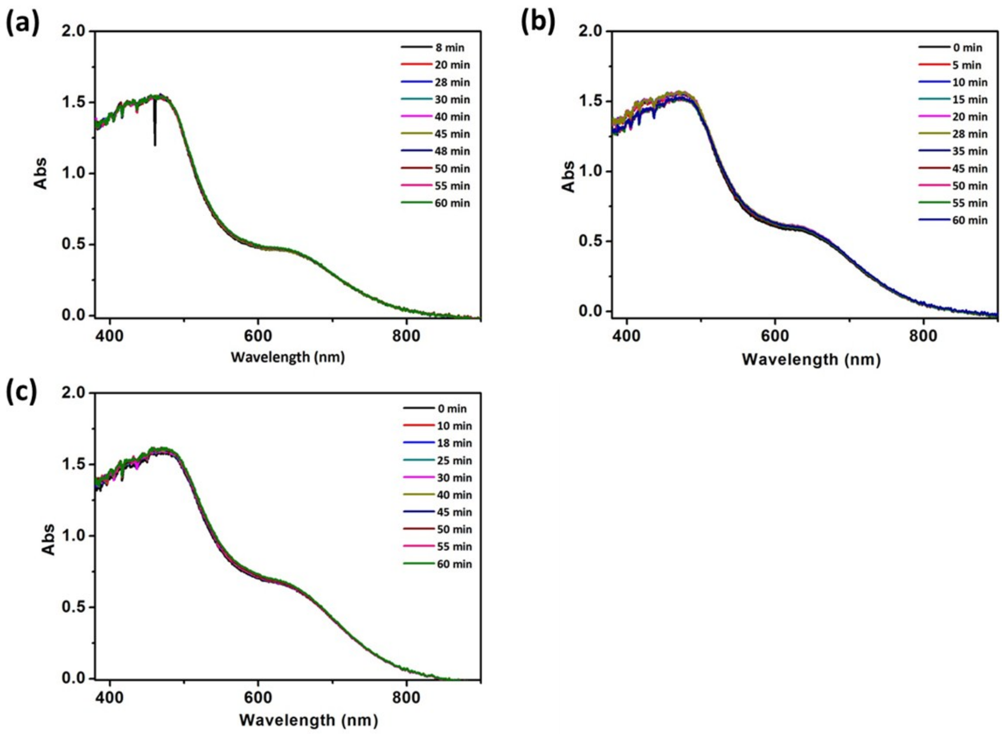

Figure S2. *In situ* UV-Vis spectroscopy of **SP-NO$_2$** over different time under high pressure of (a) 12.0 GPa; (2) 12.4 GPa; (c) 12.8 GPa.

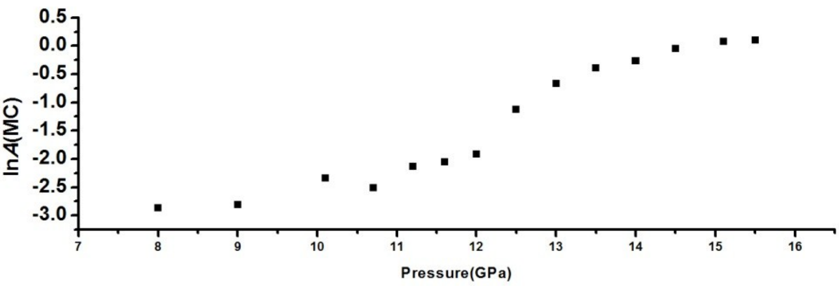

Figure S3. Correlation of ln*A*(**MC**) with pressure (P) in a pressure range of 8.0-16.0 GPa for **SP-NO$_2$**.

From the correlation, it was found that when the pressure was low, *A*(**MC**) was close to 0, and the changes of ln*A*(**MC**) was very limited and the threshold was at ca. 10 GPa. When the pressure was high enough, ln*A*(**MC**) change very slowly. Considering that ln[1/(n-n(**MC**))] cannot be approximated to be constant, and the fluctuation of optical path length of the sample under high pressure must be taken into account, the limited pressure range was chosen for further study.

2) *In situ* UV-Vis Spectra for **SP-H**

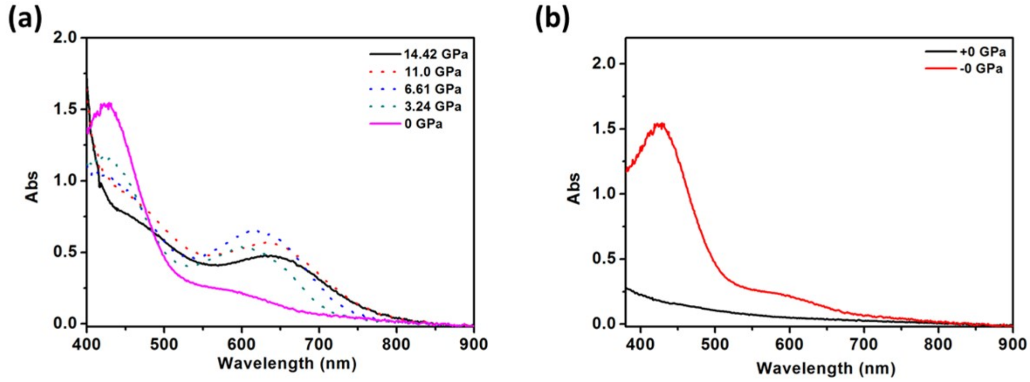

Figure S4. (a) *In situ* UV-Vis spectroscopy of **SP-H** under high pressure during decompression process in the range of 0-14.0 GPa; (b) The comparison of spectra of **SP-H** before and after the pressure treatment.

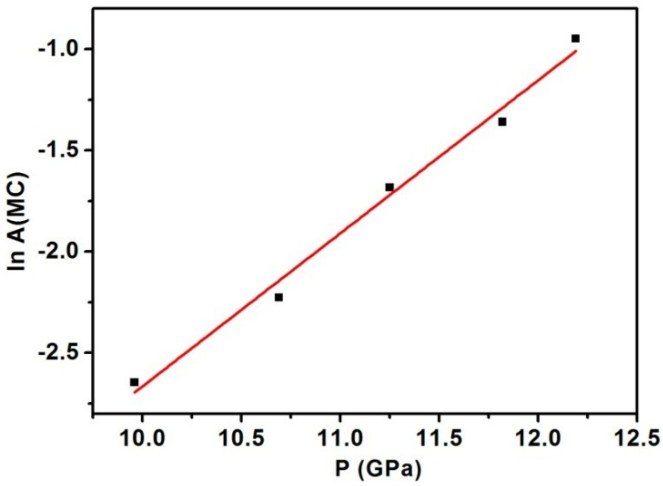

Figure S5. Correlation of lnA(**MC**) with pressure (P) in a pressure range of 10.0-13.0 GPa for **SP-H**.

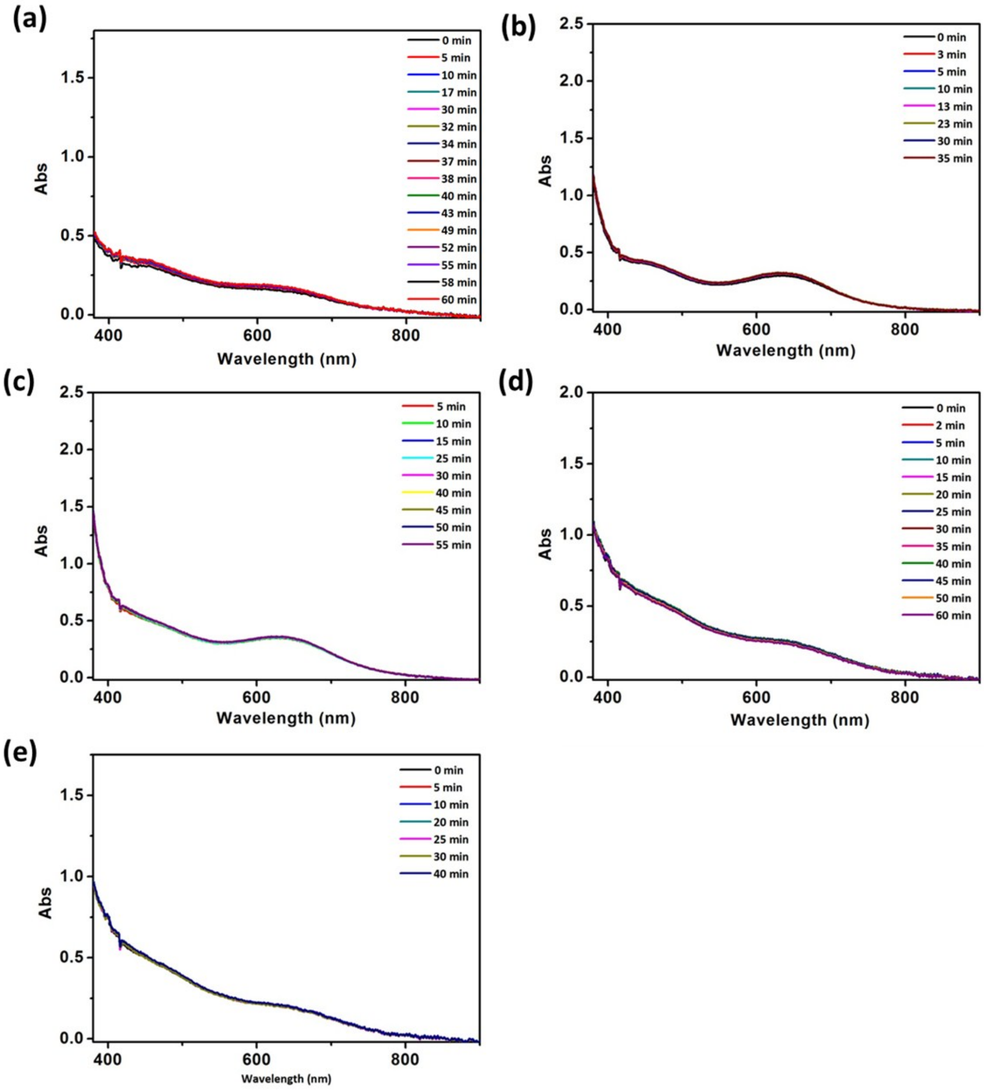

Figure S6. *In situ* UV-Vis spectroscopy of **SP-H** over different time under high pressure of (a) 11.6 GPa; (2) 11.8 GPa; (c) 12.6 GPa; (d) 13.4 GPa; (e) 13.9 GPa.

3) *In situ* UV-Vis Spectra for **SP-Ph**

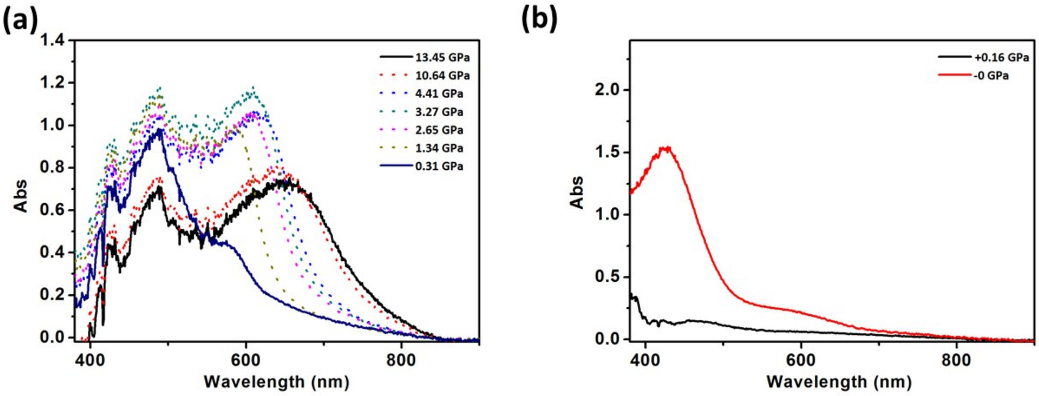

Figure S7. (a) *In situ* UV-Vis spectroscopy of **SP-Ph** under high pressure during decompression process in the range of 0-13.5 GPa; (b) The comparison of spectra of **SP-Ph** before and after the pressure treatment.

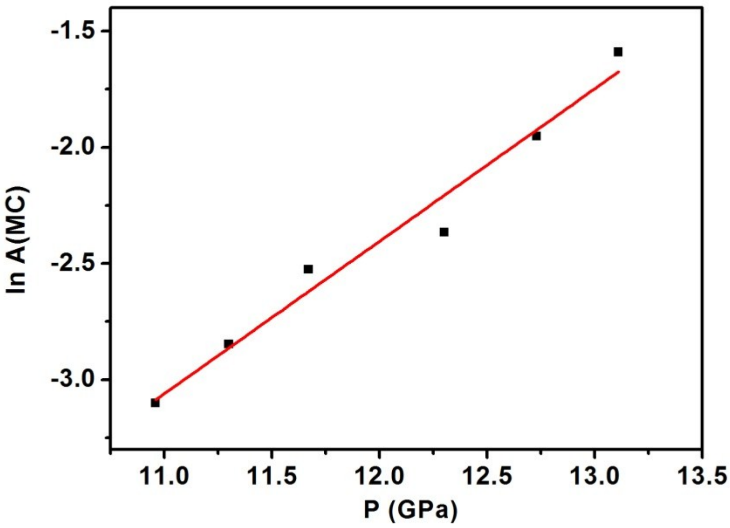

Figure S8. Correlation of lnA(**MC**) with pressure (P) in a pressure range of 10.0-14.0 GPa for **SP-Ph**.

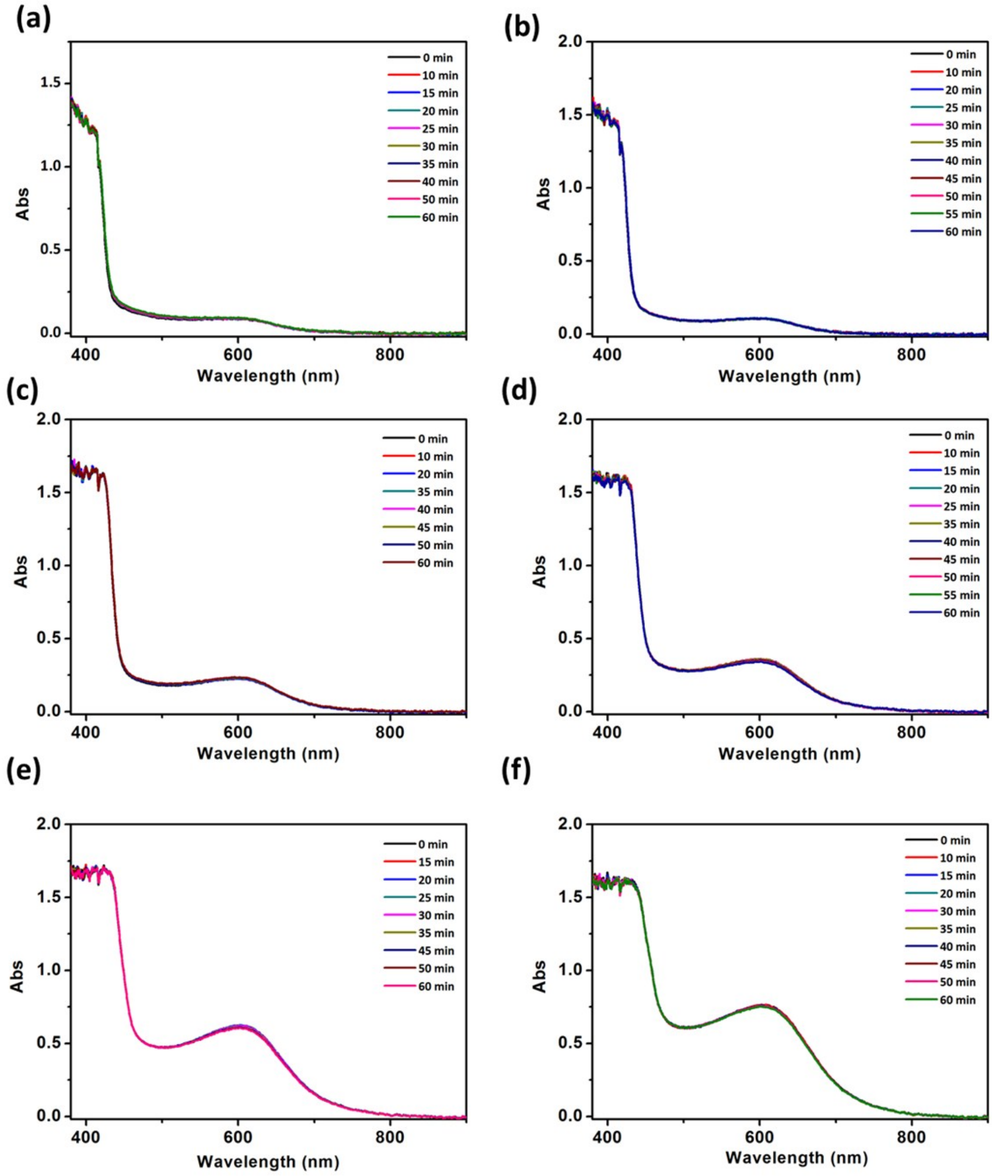

Figure S9. *In situ* UV-Vis spectroscopy of **SP-Ph** over different time under high pressure of (a) 8.8 GPa; (2) 9.3 GPa; (c) 10.7 GPa; (d) 11.0 GPa; (e) 11.4 GPa; (f) 12.0 GPa.

4) Control Experiment

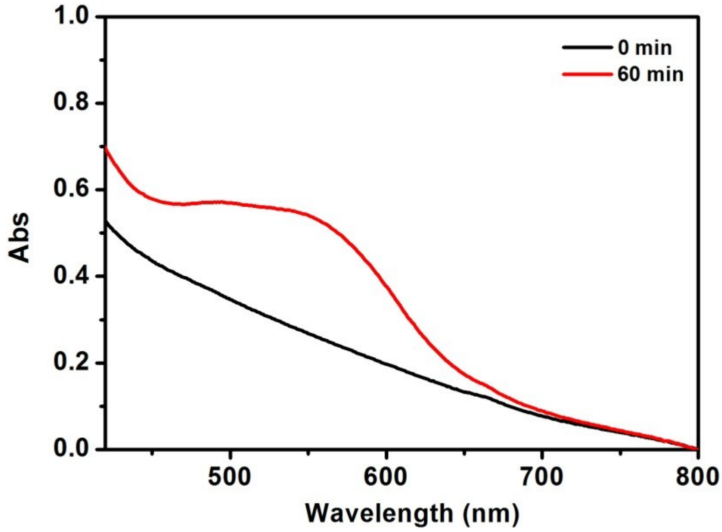

Figure S10. UV-Vis spectroscopy of **SP-NO$_2$** after UV irradiation of Hg lamp at 365 nm (500 W) treatment in 0 min and 60 min under atmospheric pressure without pressure treatment as the control experiment to compare with the products after the pressure treatment without UV radiation.

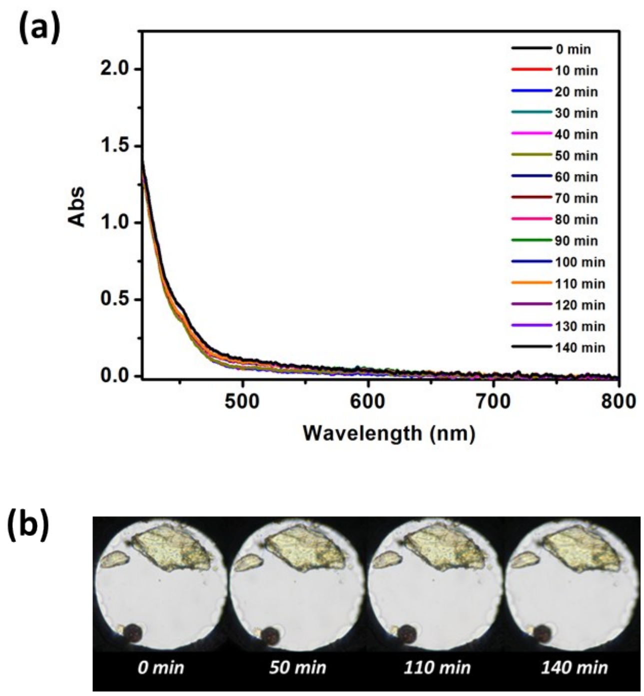

Figure S11. *In situ* (a) UV-Vis spectroscopy and (b) micrographs of **SP-NO$_2$** at different time (from 0 min to 140 min) under the pressure of 0.9 GPa.

3. Derivation of Equation

The equilibrium constant could be quantified from the fraction of **MC-NO$_2$**, which was proportional to absorbance of the characteristic absorption peak of **MC- NO$_2$**:

$$K = \frac{n(MC)}{n - n(MC)}$$

Due to the limited detection range of pressure, in order to get qualitative information and get an approximate working curve in application, ln[1/(n-n(**MC**))] is approximated to be constant and then ln***K*** is approximately proportional to the natural logarithm of percentage of **MC** form, which can be indexed by A(**MC**), absorbance of **MC** form:

$$lnK \propto lnA(MC)_{+C}$$

According to the relationship:

$$\Delta V = \left(-\frac{\partial \Delta G}{\partial P}\right)_T = (-\frac{\partial lnK}{\partial P})_T RT$$

Thus,

$$\Delta V \propto \left(-\frac{\partial lnA(MC)}{\partial P}\right)_T RT$$

Although this equation was not suitable in a larger region of pressure because of approximation, this relationship provided qualitative evidence for negative reaction volume of the isomerization process.

4. X-ray Diffraction Pattern

*The crystals of **SP-NO_2** were obtained, and its X-ray crystal structure (Scheme 1b) was found to be the same with that in the Cambridge Crystallographic Data Centre (registered without CCDC#).

Table *S1*. Crystal data and structure refinement for **SP-NO_2**.

Identification code	**SP-NO_2**	
Empirical formula	C19 H18 N2 O3	
Formula weight	322.35	
Temperature	173.1500 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 16.076(3) Å	α= 90°.
	b = 10.906(6) Å	β= 106.382(4)°.
	c = 19.607(4) Å	γ= 90°.
Volume	3298(2) $Å^3$	
Z	8	
Density (calculated)	1.298 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	1360	
Crystal size	0.32 x 0.28 x 0.1 mm^3	
Theta range for data collection	2.159 to 27.473°.	
Index ranges	-18<=h<=20, -14<=k<=14, -25<=l<=20	
Reflections collected	24340	
Independent reflections	7506 [R(int) = 0.0532]	
Completeness to theta = 26.000°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8488	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7506 / 0 / 439	
Goodness-of-fit on F^2	1.301	
Final R indices [I>2sigma(I)]	R1 = 0.0864, wR2 = 0.1574	
R indices (all data)	R1 = 0.0989, wR2 = 0.1648	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.304 and -0.239 e.$Å^{-3}$	

Table *S2*. Atomic coordinates (x10^4) and equivalent isotropic displacement parameters (Å^{2}x10^3) for **SP-NO$_2$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O1A	7912(1)	6630(2)	4037(1)	29(1)
O2A	10396(1)	8645(2)	2368(1)	44(1)
O3A	10797(1)	6747(2)	2471(1)	43(1)
N1A	6909(1)	5285(2)	4296(1)	32(1)
N2A	10336(1)	7592(2)	2566(1)	30(1)
C1A	7813(2)	5404(2)	4338(1)	27(1)
C2A	8273(2)	5427(2)	5156(1)	28(1)
C3A	7546(2)	5853(2)	5447(1)	27(1)
C4A	7563(2)	6193(2)	6130(1)	35(1)
C5A	6785(2)	6448(2)	6283(2)	40(1)
C6A	6017(2)	6363(2)	5757(2)	41(1)
C7A	5982(2)	6022(2)	5061(2)	36(1)
C8A	6763(2)	5750(2)	4920(1)	27(1)
C9A	9074(2)	6249(3)	5356(2)	44(1)
C10A	8536(2)	4120(3)	5434(2)	41(1)
C11A	6260(2)	5409(4)	3616(2)	52(1)
C12A	8122(2)	4411(2)	3940(1)	31(1)
C13A	8660(2)	4622(2)	3549(1)	31(1)
C14A	8920(2)	5857(2)	3437(1)	24(1)
C15A	9531(2)	6123(2)	3076(1)	25(1)
C16A	9688(2)	7334(2)	2942(1)	24(1)
C17A	9253(2)	8298(2)	3151(1)	28(1)
C18A	8660(2)	8045(2)	3523(1)	30(1)
C19A	8502(2)	6831(2)	3672(1)	24(1)
O1	6993(1)	1649(2)	5425(1)	37(1)
O2	5067(1)	1796(2)	7774(1)	45(1)
O3	5373(1)	3710(2)	7726(1)	45(1)
N1	8058(1)	300(2)	5255(1)	30(1)
N2	5404(1)	2650(2)	7539(1)	30(1)
C1	7139(2)	409(2)	5177(1)	29(1)
C2	6722(2)	395(2)	4352(1)	32(1)
C3	7470(2)	819(2)	4090(1)	27(1)
C4	7506(2)	1160(2)	3421(1)	36(1)

C5	8304(2)	1442(3)	3312(2)	42(1)
C6	9048(2)	1399(2)	3867(2)	40(1)
C7	9029(2)	1055(2)	4546(2)	34(1)
C8	8233(2)	747(2)	4643(1)	26(1)
C9	6467(2)	-911(3)	4078(2)	45(1)
C10	5918(2)	1221(3)	4118(2)	52(1)
C11	8664(2)	488(3)	5949(2)	53(1)
C12	6831(2)	-575(2)	5578(2)	36(1)
C13	6463(2)	-358(2)	6095(2)	35(1)
C14	6332(2)	889(2)	6301(1)	28(1)
C15	5939(2)	1166(2)	6831(1)	29(1)
C16	5846(2)	2376(2)	7000(1)	25(1)
C17	6146(2)	3336(2)	6670(1)	30(1)
C18	6536(2)	3066(2)	6142(1)	30(1)
C19	6624(2)	1850(2)	5954(1)	28(1)

Table *S3*. Bond lengths [Å] and angles [°] for **SP-NO$_2$**

O1A-C1A	1.488(3)
O1A-C19A	1.357(3)
O2A-N2A	1.225(3)
O3A-N2A	1.229(3)
N1A-C1A	1.439(3)
N1A-C8A	1.403(3)
N1A-C11A	1.450(4)
N2A-C16A	1.463(3)
C1A-C2A	1.565(3)
C1A-C12A	1.498(3)
C2A-C3A	1.511(3)
C2A-C9A	1.527(4)
C2A-C10A	1.543(4)
C3A-C4A	1.382(3)
C3A-C8A	1.391(4)
C4A-C5A	1.394(4)
C5A-C6A	1.371(4)
C6A-C7A	1.400(4)
C7A-C8A	1.392(3)
C12A-C13A	1.328(3)
C13A-C14A	1.445(3)
C14A-C15A	1.392(3)
C14A-C19A	1.404(3)
C15A-C16A	1.384(3)
C16A-C17A	1.386(3)
C17A-C18A	1.383(3)
C18A-C19A	1.395(3)
O1-C1	1.478(3)
O1-C19	1.351(3)
O2-N2	1.231(3)
O3-N2	1.218(3)
N1-C1	1.447(3)
N1-C8	1.395(3)
N1-C11	1.447(3)
N2-C16	1.462(3)
C1-C2	1.566(4)
C1-C12	1.496(3)
C2-C3	1.509(3)
C2-C9	1.536(4)
C2-C10	1.535(4)

C3-C4	1.380(3)	C3A-C4A-C5A	119.3(3)
C3-C8	1.392(3)	C6A-C5A-C4A	119.8(3)
C4-C5	1.392(4)	C5A-C6A-C7A	122.1(2)
C5-C6	1.372(4)	C8A-C7A-C6A	117.4(3)
C6-C7	1.391(4)	C3A-C8A-N1A	109.7(2)
C7-C8	1.388(3)	C3A-C8A-C7A	120.9(2)
C12-C13	1.331(3)	C7A-C8A-N1A	129.2(2)
C13-C14	1.451(4)	C13A-C12A-C1A	122.7(2)
C14-C15	1.393(3)	C12A-C13A-C14A	120.9(2)
C14-C19	1.400(3)	C15A-C14A-C13A	123.2(2)
C15-C16	1.379(3)	C15A-C14A-C19A	118.8(2)
C16-C17	1.387(3)	C19A-C14A-C13A	117.9(2)
C17-C18	1.384(3)	C16A-C15A-C14A	119.2(2)
C18-C19	1.394(3)	C15A-C16A-N2A	118.3(2)
		C15A-C16A-C17A	122.2(2)
C19A-O1A-C1A	121.49(18)	C17A-C16A-N2A	119.5(2)
C1A-N1A-C11A	119.8(2)	C18A-C17A-C16A	119.0(2)
C8A-N1A-C1A	109.4(2)	C17A-C18A-C19A	119.6(2)
C8A-N1A-C11A	121.0(2)	O1A-C19A-C14A	121.5(2)
O2A-N2A-O3A	123.4(2)	O1A-C19A-C18A	117.3(2)
O2A-N2A-C16A	118.1(2)	C18A-C19A-C14A	121.1(2)
O3A-N2A-C16A	118.5(2)	C19-O1-C1	123.11(19)
O1A-C1A-C2A	108.61(19)	C1-N1-C11	119.0(2)
O1A-C1A-C12A	110.83(18)	C8-N1-C1	109.1(2)
N1A-C1A-O1A	106.11(19)	C8-N1-C11	120.9(2)
N1A-C1A-C2A	103.72(18)	O2-N2-C16	118.1(2)
N1A-C1A-C12A	112.5(2)	O3-N2-O2	123.1(2)
C12A-C1A-C2A	114.5(2)	O3-N2-C16	118.8(2)
C3A-C2A-C1A	101.6(2)	O1-C1-C2	106.7(2)
C3A-C2A-C9A	114.1(2)	O1-C1-C12	112.11(19)
C3A-C2A-C10A	108.3(2)	N1-C1-O1	107.0(2)
C9A-C2A-C1A	113.2(2)	N1-C1-C2	103.67(19)
C9A-C2A-C10A	109.0(2)	N1-C1-C12	111.4(2)
C10A-C2A-C1A	110.5(2)	C12-C1-C2	115.3(2)
C4A-C3A-C2A	130.0(2)	C3-C2-C1	101.5(2)
C4A-C3A-C8A	120.5(2)	C3-C2-C9	108.9(2)
C8A-C3A-C2A	109.2(2)	C3-C2-C10	113.7(2)

C9-C2-C1	111.5(2)
C10-C2-C1	112.5(2)
C10-C2-C9	108.7(2)
C4-C3-C2	131.2(2)
C4-C3-C8	119.5(2)
C8-C3-C2	109.1(2)
C3-C4-C5	119.5(3)
C6-C5-C4	120.3(3)
C5-C6-C7	121.2(3)
C8-C7-C6	117.9(3)
C3-C8-N1	110.1(2)
C7-C8-N1	128.4(2)
C7-C8-C3	121.5(2)
C13-C12-C1	123.9(2)
C12-C13-C14	120.6(2)
C15-C14-C13	122.9(2)
C15-C14-C19	119.0(2)
C19-C14-C13	118.1(2)
C16-C15-C14	119.3(2)
C15-C16-N2	118.5(2)
C15-C16-C17	122.3(2)
C17-C16-N2	119.2(2)
C18-C17-C16	118.6(2)
C17-C18-C19	120.1(2)
O1-C19-C14	122.1(2)
O1-C19-C18	117.2(2)
C18-C19-C14	120.7(2)

Table *S4*. Anisotropic displacement parameters ($Å^2x10^3$) for **SP-NO$_2$**. The anisotropic displacement factor exponent takes the form: -2^2[h^2 $a^{*2}U^{11}$ + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O1A	36(1)	25(1)	34(1)	1(1)	21(1)	2(1)
O2A	57(1)	33(1)	54(1)	8(1)	36(1)	-3(1)
O3A	48(1)	36(1)	59(1)	-4(1)	38(1)	2(1)
N1A	28(1)	40(1)	29(1)	0(1)	11(1)	-5(1)
N2A	36(1)	30(1)	27(1)	-4(1)	16(1)	-4(1)
C1A	30(1)	25(1)	29(1)	1(1)	17(1)	-4(1)
C2A	31(1)	28(1)	28(1)	1(1)	13(1)	-1(1)
C3A	32(1)	24(1)	32(1)	2(1)	18(1)	0(1)
C4A	47(2)	29(1)	33(1)	1(1)	18(1)	-2(1)
C5A	63(2)	27(1)	43(2)	1(1)	37(2)	2(1)
C6A	50(2)	26(1)	65(2)	7(1)	45(2)	6(1)
C7A	29(1)	32(1)	51(2)	7(1)	20(1)	0(1)
C8A	30(1)	23(1)	34(1)	4(1)	16(1)	0(1)
C9A	32(1)	62(2)	37(2)	-4(1)	11(1)	-9(1)
C10A	39(2)	46(2)	42(2)	7(1)	18(1)	10(1)
C11A	38(2)	79(2)	36(2)	-9(2)	5(1)	-9(2)
C12A	44(2)	22(1)	34(1)	-2(1)	21(1)	-4(1)
C13A	41(1)	24(1)	34(1)	-4(1)	21(1)	2(1)

C14A	31(1)	22(1)	21(1)	1(1)	10(1)	1(1)
C15A	28(1)	26(1)	23(1)	-4(1)	11(1)	2(1)
C16A	28(1)	27(1)	21(1)	-1(1)	11(1)	-2(1)
C17A	35(1)	23(1)	28(1)	2(1)	14(1)	-2(1)
C18A	37(1)	25(1)	33(1)	-2(1)	20(1)	3(1)
C19A	26(1)	25(1)	24(1)	-1(1)	12(1)	0(1)
O1	57(1)	25(1)	43(1)	1(1)	38(1)	-1(1)
O2	65(1)	35(1)	50(1)	1(1)	42(1)	-5(1)
O3	69(1)	31(1)	47(1)	-11(1)	36(1)	-4(1)
N1	31(1)	34(1)	26(1)	3(1)	10(1)	3(1)
N2	37(1)	28(1)	27(1)	1(1)	15(1)	-1(1)
C1	38(1)	22(1)	34(1)	-1(1)	21(1)	1(1)
C2	28(1)	34(1)	34(1)	-1(1)	12(1)	0(1)
C3	32(1)	24(1)	25(1)	-3(1)	10(1)	1(1)
C4	51(2)	32(1)	25(1)	0(1)	12(1)	1(1)
C5	70(2)	33(2)	37(2)	-2(1)	36(2)	-3(1)
C6	49(2)	27(1)	58(2)	-1(1)	39(2)	0(1)
C7	30(1)	30(1)	46(2)	-3(1)	17(1)	2(1)
C8	29(1)	22(1)	29(1)	-1(1)	14(1)	4(1)
C9	45(2)	44(2)	47(2)	-6(1)	16(1)	-12(1)
C10	36(2)	61(2)	59(2)	12(2)	12(2)	12(2)
C11	51(2)	71(2)	30(2)	9(2)	1(1)	-1(2)
C12	53(2)	22(1)	44(2)	1(1)	30(1)	1(1)
C13	51(2)	23(1)	41(2)	3(1)	29(1)	-3(1)
C14	36(1)	25(1)	28(1)	1(1)	17(1)	0(1)
C15	36(1)	27(1)	28(1)	4(1)	17(1)	-1(1)
C16	28(1)	28(1)	22(1)	1(1)	13(1)	-1(1)
C17	40(1)	22(1)	32(1)	0(1)	18(1)	-2(1)
C18	42(2)	21(1)	35(1)	3(1)	23(1)	-2(1)
C19	33(1)	27(1)	28(1)	2(1)	17(1)	0(1)

Table *S5*. Hydrogen coordinates (x10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **SP-NO$_2$**.

	x	y	z	U(eq)
H4A	8087	6251	6483	42
H5A	6788	6675	6741	48
H6A	5503	6539	5866	50

H7A	5457	5978	4707	43
H9AA	9478	5981	5109	65
H9AB	9340	6203	5860	65
H9AC	8906	7081	5226	65
H10A	8045	3583	5281	61
H10B	8732	4131	5944	61
H10C	8994	3830	5250	61
H11A	6172	6262	3496	78
H11B	5725	5052	3643	78
H11C	6454	4995	3256	78
H12A	7928	3614	3969	38
H13A	8873	3967	3346	37
H15A	9830	5494	2928	30
H17A	9359	9102	3042	33
H18A	8367	8680	3673	35
H4	7002	1202	3046	43
H5	8333	1661	2861	51
H6	9575	1604	3788	48
H7	9533	1032	4922	41
H9A	5991	-1188	4242	67
H9B	6953	-1450	4252	67
H9C	6298	-910	3567	67
H10D	6089	2062	4207	78
H10E	5517	1008	4380	78
H10F	5646	1108	3619	78
H11D	8444	109	6305	80
H11E	8738	1351	6044	80
H11F	9213	128	5960	80
H12	6901	-1387	5460	44
H13	6287	-1011	6326	42
H15	5741	542	7068	34
H17	6087	4144	6801	36
H18	6740	3696	5913	36

Table S6. Torsion angles [°] for **SP-NO_2**.

O1A-C1A-C2A-C3A	89.4(2)
O1A-C1A-C2A-C9A	-33.3(3)

O1A-C1A-C2A-C10A	-155.86(19)
O1A-C1A-C12A-C13A	20.6(4)
O2A-N2A-C16A-C15A	170.9(2)
O2A-N2A-C16A-C17A	-9.0(3)
O3A-N2A-C16A-C15A	-9.9(3)
O3A-N2A-C16A-C17A	170.2(2)
N1A-C1A-C2A-C3A	-23.2(2)
N1A-C1A-C2A-C9A	-145.9(2)
N1A-C1A-C2A-C10A	91.6(2)
N1A-C1A-C12A-C13A	139.2(3)
N2A-C16A-C17A-C18A	-178.3(2)
C1A-O1A-C19A-C14A	13.1(3)
C1A-O1A-C19A-C18A	-168.6(2)
C1A-N1A-C8A-C3A	-16.5(3)
C1A-N1A-C8A-C7A	167.4(2)
C1A-C2A-C3A-C4A	-171.6(3)
C1A-C2A-C3A-C8A	14.5(3)
C1A-C12A-C13A-C14A	-5.5(4)
C2A-C1A-C12A-C13A	-102.7(3)
C2A-C3A-C4A-C5A	-174.1(2)
C2A-C3A-C8A-N1A	0.1(3)
C2A-C3A-C8A-C7A	176.5(2)
C3A-C4A-C5A-C6A	-0.3(4)
C4A-C3A-C8A-N1A	-174.5(2)
C4A-C3A-C8A-C7A	1.9(4)
C4A-C5A-C6A-C7A	0.2(4)
C5A-C6A-C7A-C8A	0.8(4)
C6A-C7A-C8A-N1A	173.7(2)
C6A-C7A-C8A-C3A	-1.9(4)
C8A-N1A-C1A-O1A	-89.4(2)
C8A-N1A-C1A-C2A	24.9(3)
C8A-N1A-C1A-C12A	149.2(2)
C8A-C3A-C4A-C5A	-0.8(4)
C9A-C2A-C3A-C4A	-49.5(4)
C9A-C2A-C3A-C8A	136.6(2)
C10A-C2A-C3A-C4A	72.0(3)
C10A-C2A-C3A-C8A	-101.9(2)

C11A-N1A-C1A-O1A	56.7(3)
C11A-N1A-C1A-C2A	171.1(2)
C11A-N1A-C1A-C12A	-64.6(3)
C11A-N1A-C8A-C3A	-162.2(2)
C11A-N1A-C8A-C7A	21.7(4)
C12A-C1A-C2A-C3A	-146.2(2)
C12A-C1A-C2A-C9A	91.1(3)
C12A-C1A-C2A-C10A	-31.4(3)
C12A-C13A-C14A-C15A	175.1(3)
C12A-C13A-C14A-C19A	-8.2(4)
C13A-C14A-C15A-C16A	174.7(2)
C13A-C14A-C19A-O1A	4.3(3)
C13A-C14A-C19A-C18A	-173.9(2)
C14A-C15A-C16A-N2A	179.7(2)
C14A-C15A-C16A-C17A	-0.4(4)
C15A-C14A-C19A-O1A	-178.8(2)
C15A-C14A-C19A-C18A	2.9(4)
C15A-C16A-C17A-C18A	1.8(4)
C16A-C17A-C18A-C19A	-0.9(4)
C17A-C18A-C19A-O1A	-179.8(2)
C17A-C18A-C19A-C14A	-1.5(4)
C19A-O1A-C1A-N1A	-146.7(2)
C19A-O1A-C1A-C2A	102.3(2)
C19A-O1A-C1A-C12A	-24.3(3)
C19A-C14A-C15A-C16A	-2.0(3)
O1-C1-C2-C3	89.4(2)
O1-C1-C2-C9	-154.8(2)
O1-C1-C2-C10	-32.5(3)
O1-C1-C12-C13	0.5(4)
O2-N2-C16-C15	-6.2(3)
O2-N2-C16-C17	172.9(2)
O3-N2-C16-C15	175.0(2)
O3-N2-C16-C17	-5.9(4)
N1-C1-C2-C3	-23.3(2)
N1-C1-C2-C9	92.4(2)
N1-C1-C2-C10	-145.2(2)
N1-C1-C12-C13	120.4(3)

N2-C16-C17-C18	-177.7(2)
C1-O1-C19-C14	-1.5(4)
C1-O1-C19-C18	179.1(2)
C1-N1-C8-C3	-17.0(3)
C1-N1-C8-C7	165.2(2)
C1-C2-C3-C4	-170.2(3)
C1-C2-C3-C8	14.4(3)
C1-C12-C13-C14	0.3(5)
C2-C1-C12-C13	-121.9(3)
C2-C3-C4-C5	-175.8(3)
C2-C3-C8-N1	0.5(3)
C2-C3-C8-C7	178.4(2)
C3-C4-C5-C6	-1.0(4)
C4-C3-C8-N1	-175.6(2)
C4-C3-C8-C7	2.4(4)
C4-C5-C6-C7	1.1(4)
C5-C6-C7-C8	0.5(4)
C6-C7-C8-N1	175.3(2)
C6-C7-C8-C3	-2.2(4)
C8-N1-C1-O1	-87.3(2)
C8-N1-C1-C2	25.3(3)
C8-N1-C1-C12	149.9(2)
C8-C3-C4-C5	-0.7(4)
C9-C2-C3-C4	72.2(4)
C9-C2-C3-C8	-103.2(2)
C10-C2-C3-C4	-49.1(4)
C10-C2-C3-C8	135.4(3)
C11-N1-C1-O1	57.2(3)
C11-N1-C1-C2	169.8(2)
C11-N1-C1-C12	-65.7(3)
C11-N1-C8-C3	-160.7(3)
C11-N1-C8-C7	21.6(4)
C12-C1-C2-C3	-145.3(2)
C12-C1-C2-C9	-29.6(3)
C12-C1-C2-C10	92.8(3)
C12-C13-C14-C15	179.1(3)
C12-C13-C14-C19	-1.6(4)

C13-C14-C15-C16	179.4(3)
C13-C14-C19-O1	2.3(4)
C13-C14-C19-C18	-178.4(3)
C14-C15-C16-N2	177.8(2)
C14-C15-C16-C17	-1.2(4)
C15-C14-C19-O1	-178.4(2)
C15-C14-C19-C18	0.9(4)
C15-C16-C17-C18	1.3(4)
C16-C17-C18-C19	-0.2(4)
C17-C18-C19-O1	178.6(2)
C17-C18-C19-C14	-0.9(4)
C19-O1-C1-N1	-122.3(2)
C19-O1-C1-C2	127.2(2)
C19-O1-C1-C12	0.1(3)
C19-C14-C15-C16	0.1(4)