9-Iodophenalenone and 9-Trifluoromethanesulfonyloxyphenalenone: Convenient Entry Points to New Phenalenones Functionalized in 9-Position. Iodine-Carbonyl Interactions Studies by X-Ray Crystallography

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Supporting Information

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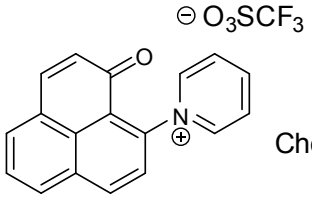
Synthesis of 1-(1-oxo-1*H*-phenalen-9-yl)pyridinium triflate

To a cooled solution of 100 mg (0.5 mmol; 1 eq) of 9-hydroxy-1*H*-phenalen-1-one in 5ml of pyridine, 0.1 ml (0.6 mmol; 1.2 eq) of triflic anhydride was added dropwise while stirring under argon atmosphere. After 5 minutes the ice bath was removed and the reaction was stirred for 4 h. Then 10 ml of H_2O was added and extraction using diethylether (3 x 15 ml) was carried out. The brown aqueous layer was left in a beaker in the fumehood over night. The next day the brown solid was washed with 50 ml of H_2O giving the product in a yield of 51% (106 mg, 0.3 mmol).



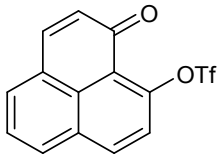
Chemical Formula: $C_{19}H_{12}F_3NO_4S$
Molecular Weight: 407,36

^{1}H-NMR (400 MHz; CD_3CN) δ 6.53 (d, *J* = 9.8 Hz, 1H), 7.89 (t, *J* = 8.3 Hz, 2H), 7.96 (d, *J* = 9.8 Hz, 1H), 8.27 – 8.20 (m, 2H), 8.33 (d, *J* = 8.4 Hz, 1H), 6.53 (d, *J* = 9.8 Hz, 1H), 8.79 (tt, *J* = 7.9, 1.4 Hz, 1H), 6.53 (d, J = 9.8 Hz, 2H). ^{13}C-NMR (100 MHz; CD_3CN) δ 120.51 & 123.70 ($J_{C,F}$ = 320 Hz), 122.81, 126.61, 128.31, 129.30 (2C), 129.84, 130.29, 133.57, 134.79, 135.45, 138.04, 142.59, 143.41, 146.17, 148.53, 184.66 (*one quaternary carbon could not be observed, possibly due to signal overlap*). UV (in MeCN) – λmax [nm] (log ε): 300 (3.84), 358 (3.95), 388 (3.94). IR (ATIR) ν_{max} 3124-3065 ($CH_{aromatics}$, weak), 1640, 1628 (C=O, sharp & intense), 1579, 1559, 1474, 1346 (S=O, slightly broad & intense), 1256, 1239, 1224, 1156 (S=O, slightly broad & intense), 1131, 1118, 1028 (CF_3, sharp & intense), 963. MS (FAB+) m/z (rel. intensity): 259 (36), 258 (100), 180 (27), 154 (13), 138 (5), 40 (25). HRMS calcd for $C_{18}H_{12}ON$: 258.0919, found: 258.0916. Melting point: 172 °C.

Synthesis of 9-trifluoromethanesulfonyloxy-1*H*-phenalen-1-one

In a round bottom flask, 500 mg (2.5 mmol; 1 eq) of 9-hydroxy-1*H*-phenalen-1-one were dissolved in 50 ml of toluene. Then 50 ml of an aqueous K_3PO_4 solution (30% (w/w)) was added and the flask was placed in a NaCl/ice bath. While stirring, 0.52 ml (3.1 mmol; 1.2 eq) of triflic anhydride was added dropwise to the mixed bilayer. After 5 minutes the ice bath was removed and the reaction was stirred for 1 h. The organic layer was separated via separation funnel. Using 20

ml of toluene the aqueous layer was extracted once and combined with the organic layer. After rotary evaporation under vacuum pressure and purification via column chromatography using diethylether as eluent, the product was obtained as pale yellow crystals in a yield of 80% (710 mg; 2.2 mmol).

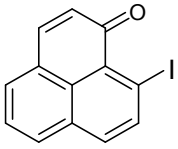


Chemical Formula: $C_{14}H_7F_3O_4S$
Molecular Weight: 328,26

^{1}H-NMR (400 MHz; $CDCl_3$) δ 6.72 (d, *J* = 9.8 Hz, 1H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.69 (dd, *J* = 8.2, 7.1 Hz, 1H), 7.73 (d, *J* = 9.8 Hz, 1H), 7.84 (d, *J* = 6.9 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 1H), 8.27 (d, *J* = 8.9 Hz, 1H). ^{13}C-NMR (100 MHz; $CDCl_3$) δ 115.28-122.93 (quartet, $J_{C,F}$ = 317 Hz, CF_3), 120.98, 122.42, 127.83, 128.55, 130.09, 131.80, 131.82, 132.82, 132.80, 136.83, 140.93, 149.62, 183.43. ^{19}F NMR ($CDCl_3$) δ -73.79 (s).UV (in MeCN) – λmax [nm] (log ε): 307 (3.57), 354 (3.96), 382 (3.86). IR (ATIR) ν_{max} 3058 ($CH_{aromatic}$, weak), 1636 (C=O, sharp & intense), 1588, 1577, 1569, 1506, 1422, 1401, 1364, 1348, 1243, 1219, 1199, 1180, 1168, 1139, 1123, 1102, 1070. MS (EI+) m/z (rel. intensity): 378 (90), 264 (12), 236 (41), 195 (38), 167 (34), 139 (100), 69 (10), 44 (4). HRMS calcd for $C_{14}H_7F_3O_4S$: 328.0017, found: 328.0013. Melting point: 108 °C.

Synthesis of 9-Iodo-1*H*-phenalen-1-one

In a round bottom flask, 300 mg (0.9 mmol; 1 eq) of 9-trifluoromethanesulfonyloxy-1*H*-phenalen-1-one and 758 mg (4.6 mmol; 5 eq) of KI were combined in 5 ml of dry DMF. The mixture was heated at 80 °C under argon atmosphere over night. The next day, the reaction was diluted with 100 ml of H_2O. The product was extracted with diethylether (4 * 50 ml), washed with H_2O (4 * 50 ml) and 30 ml of saturated NaCl solution. Afterwards, the ether solution was dried over Na_2SO_4 and evaporated via rotary evaporation. A column chromatography was carried out using DCM as eluent yielding the desired product as orange crystals in a yield of 69% (193 mg; 0.6 mmol).



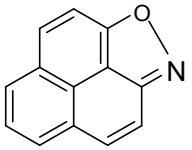
Chemical Formula: $C_{13}H_7IO$
Molecular Weight: 306,10

^{1}H-NMR (500 MHz; $CDCl_3$) δ 6.79 (d, *J* = 9.7 Hz, 1H), 7.61 (dd, *J* = 8.1, 7.1 Hz, 1H), 7.66 (d, *J* = 9.7 Hz, 1H), 7.70 (d, *J* = 8.6 Hz, 1H), 7.70 (d, *J* = 6.9 Hz, 1H), 7.97 (dd, *J* = 8.2, 0.9 Hz, 1H), 8.37 (d, *J* = 8.5 Hz, 1H). ^{13}C-NMR (125 MHz; $CDCl_3$) δ 100.25, 126.94, 127.23, 128.49, 128.71, 129.28, 131.54, 131.98, 132.42, 133.97, 140.01, 142.24, 183.49. UV (in MeCN) – λmax [nm] (log

ε): 307 (3.74), 365 (4.33), 384 (3.91). IR (ATIR) ν_{max} 3033 ($CH_{aromatic}$, weak), 1623 (C=O, sharp & intense), 1572, 1548, 1487, 1427, 1401, 1353, 1331, 1256, 1243, 1182, 1126, 1090, 1046, 1000. MS (EI+) m/z (rel. intensity): 306 (100), 278 (16), 151 (73), 150 (29), 84 (14), 75 (6). 49 (13). HRMS calcd for $C_{13}H_7IO$: 305.9542, found: 305.9546. Melting point: 122 °C.

Synthesis of phenaleno[1,9-*cd*]isoxazole

In a round bottom flask, 100 mg (0.3 mmol; 1 eq) of 1-oxo-1*H*-phenalen-9-yl trifluoromethanesulfonate and 100 mg (1.5 mmol; 5 eq) of NaN_3 were mixed in 10 ml of DMF. Under argon atmosphere, the reaction was stirred at room temperature for 72 h. The solution was diluted with 100 ml of H_2O and subsequently extracted with diethylether (4 * 30 ml). After washing with H_2O (3 * 50 ml) and 30 ml of saturated NaCl solution, the ether solution was dried over Na_2SO_4. The solvent was removed via rotary evaporation yielding the desired product as yellow crystals in a yield of 90% (53 mg; 0.3 mmol).



Chemical Formula: $C_{13}H_7NO$
Molecular Weight: 193,20

^{1}H-NMR (400 MHz; $CDCl_3$) δ 7.73 (d, *J* = 9.4 Hz, 1H), 7.90 (dd, *J* = 8.1, 7.4 Hz, 1H), 7.95 (d, *J* = 9.0 Hz, 1H), 7.99 (d, *J* = 9.4 Hz, 1H), 8.13 (d, *J* = 7.4 Hz, 1H), 8.24 (d, *J* = 9.0 Hz, 1H), 8.27 (d, *J* = 8.1 Hz, 1H). ^{13}C-NMR (100 MHz; $CDCl_3$) δ 111.89, 115.42, 117.45, 122.90, 126.57, 127.31, 127.67, 128.09, 128.17, 130.30, 134.43, 153.59, 161.21. UV (in MeCN) – λmax [nm] (log ε): 314 (4.08), 328 (4.24), 350 (3.88). IR (ATIR) ν_{max} 3035 ($CH_{aromatic}$, weak), 1695, 1633, 1617, 1577, 1550, 1495, 1475, 1458, 1412, 1344, 1317, 1237, 1219, 1181, 1142, 1115, 1001. . MS (EI+) m/z (rel. intensity): 193 (100), 164 (31), 138 (18), 137 (8), 111 (3), 87 (4), 83 (5), 63 (3), 40 (3). HRMS calcd for $C_{13}H_7NO$: 193.0528, found: 193.0527. Melting point: 176 °C

NMR spectra

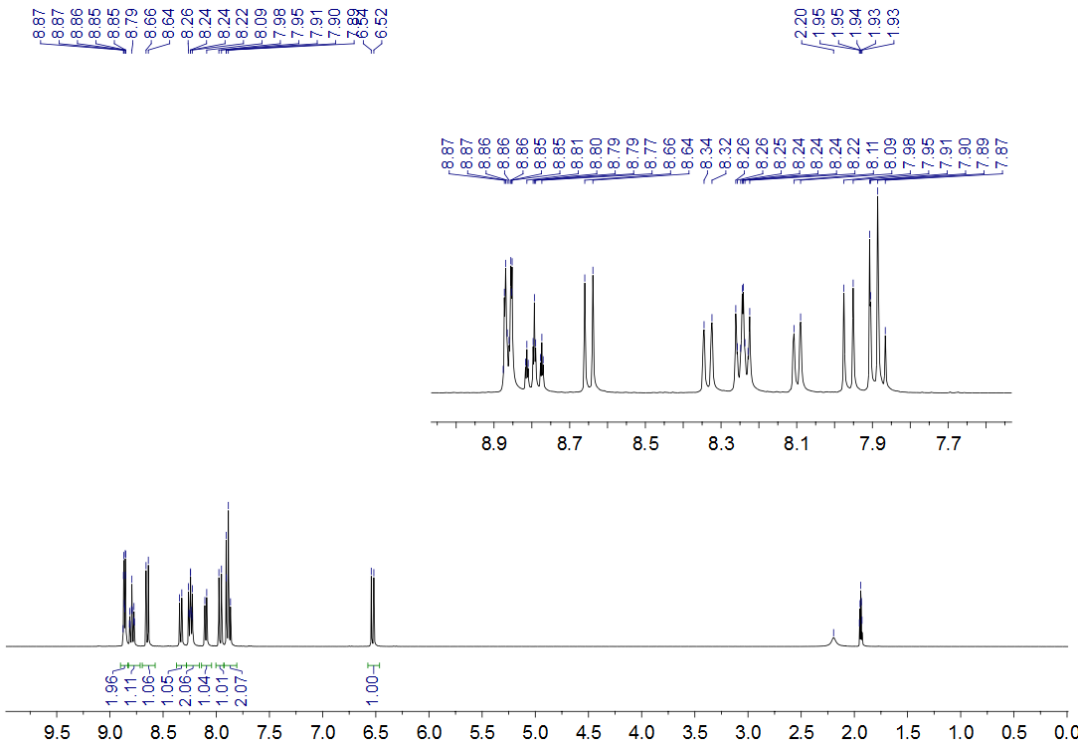


Figure 1 ^{1}H-NMR spectrum (400 MHz; CD_3CN) of 1-(1-Oxo-1*H*-phenalen-9-yl)pyridinium triflate.

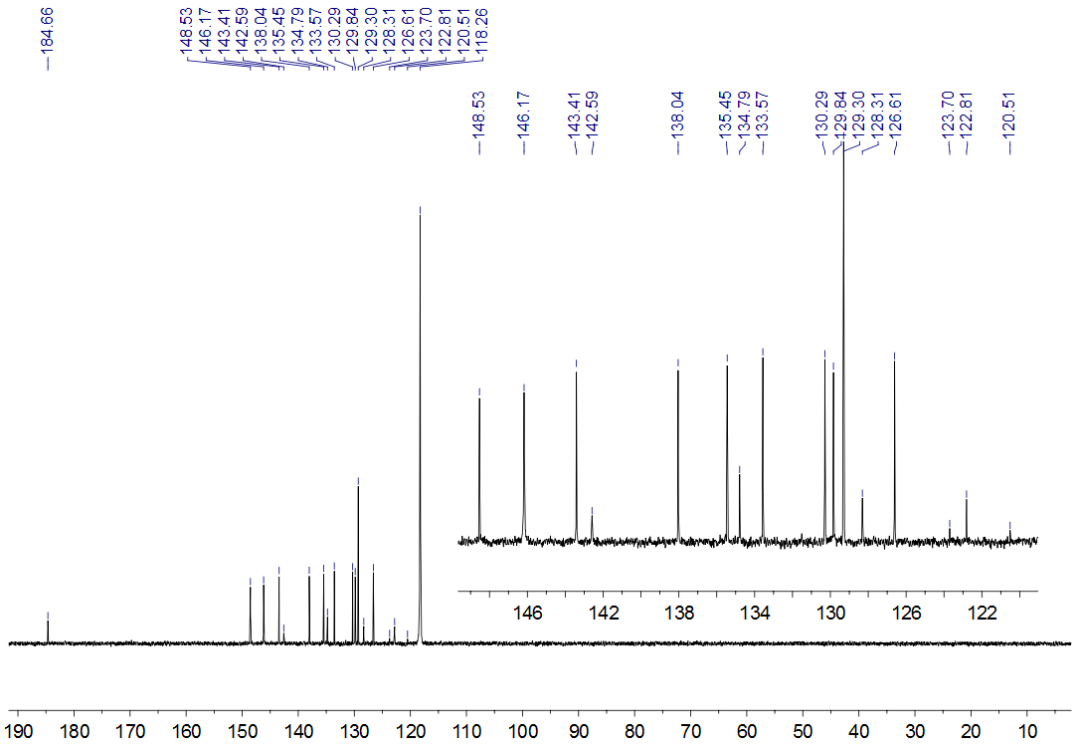


Figure 2 ^{13}C-NMR spectrum (100 MHz; CD_3CN) of 1-(1-Oxo-1*H*-phenalen-9-yl)pyridinium triflate.

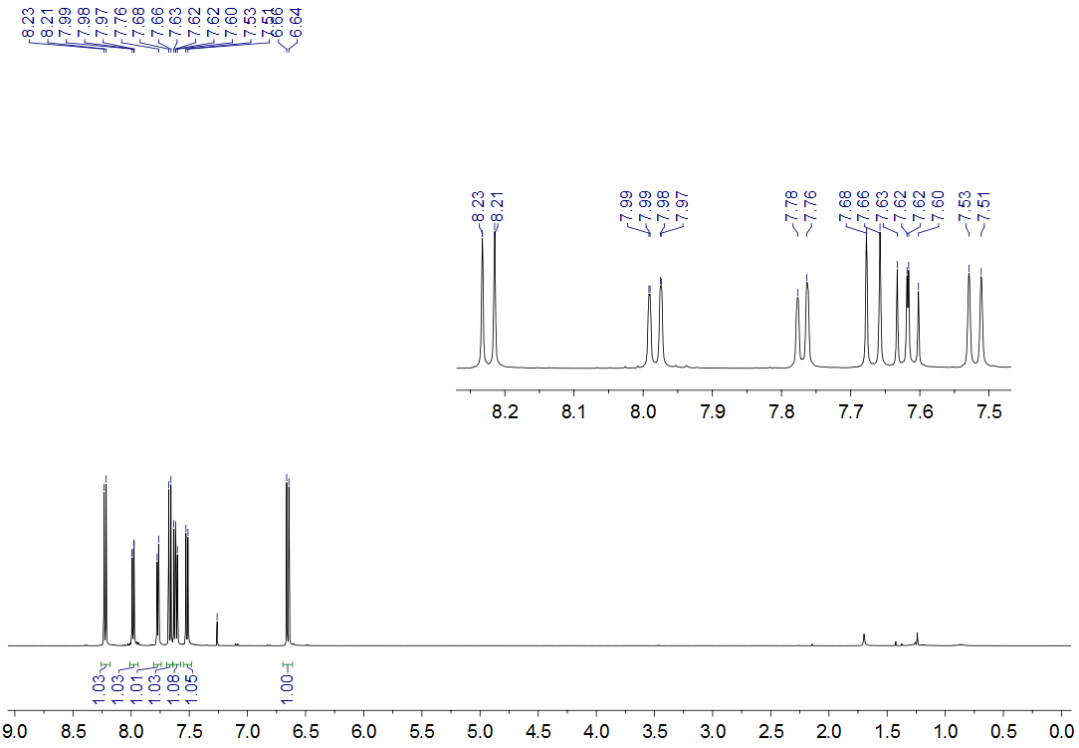


Figure 3 ^{1}H-NMR spectrum (400 MHz; $CDCl_3$) of 9-trifluoromethanesulfonyloxy-1*H*-phenalen-1-one.

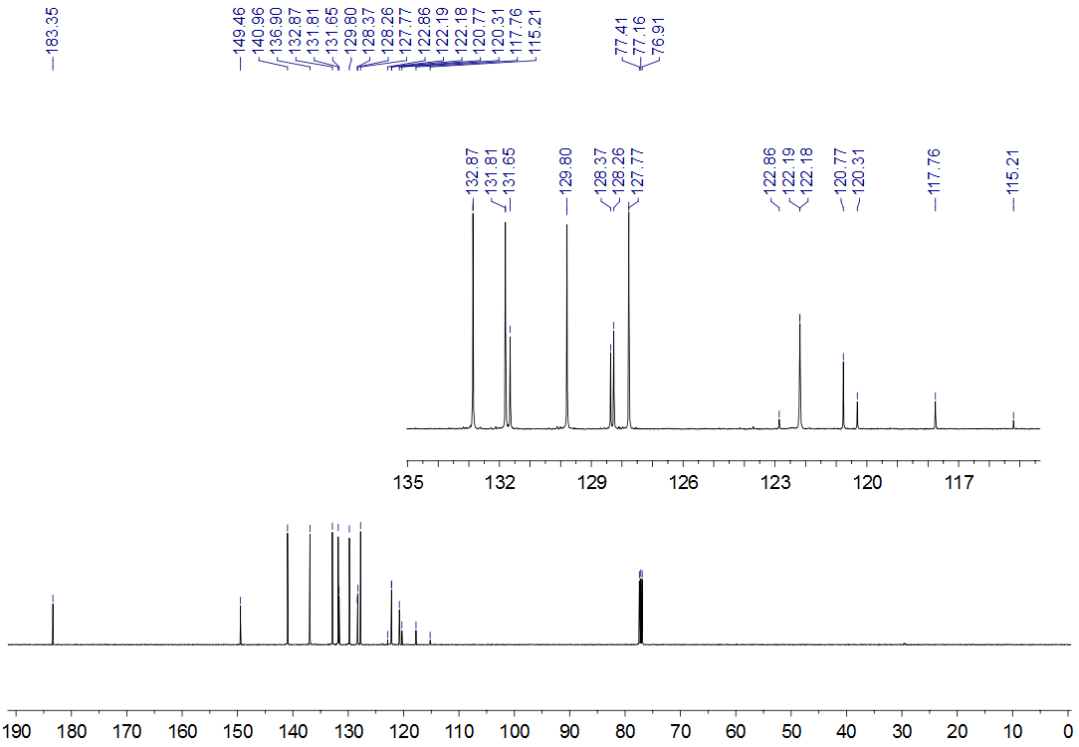


Figure 4 ^{13}C-NMR spectrum (100 MHz; $CDCl_3$) of 9-trifluoromethanesulfonyloxy-1*H*-phenalen-1-one.

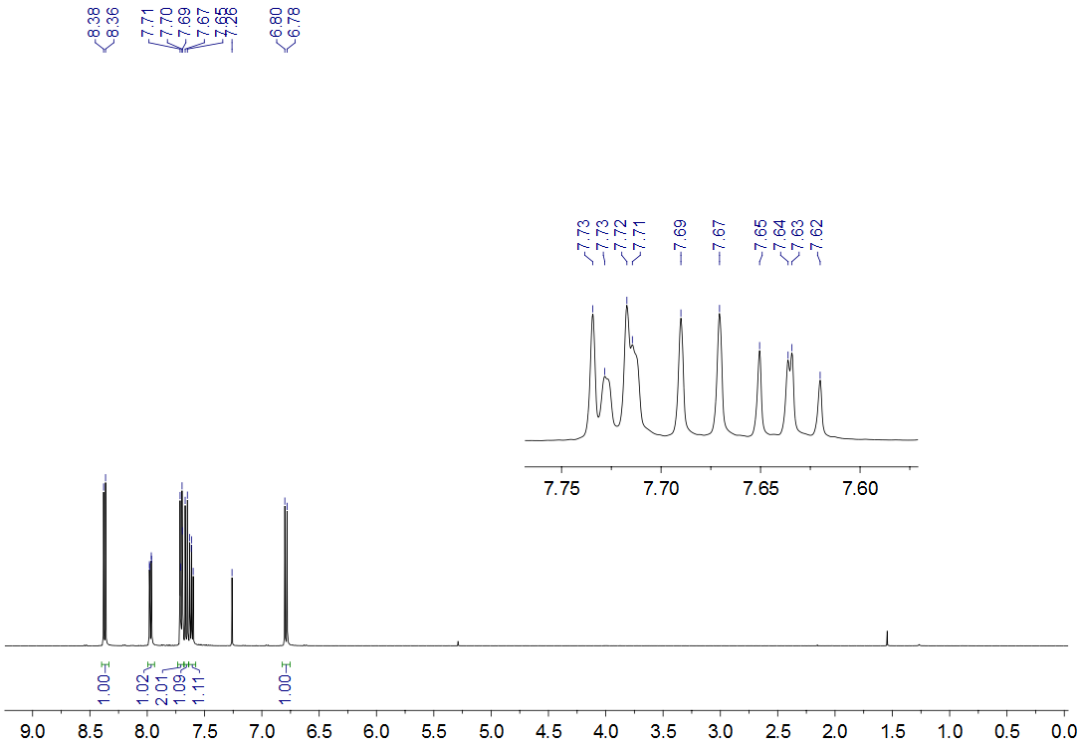


Figure 5 ^{1}H-NMR spectrum (500 MHz; $CDCl_3$) of 9-iodo-1*H*-phenalen-1-one.

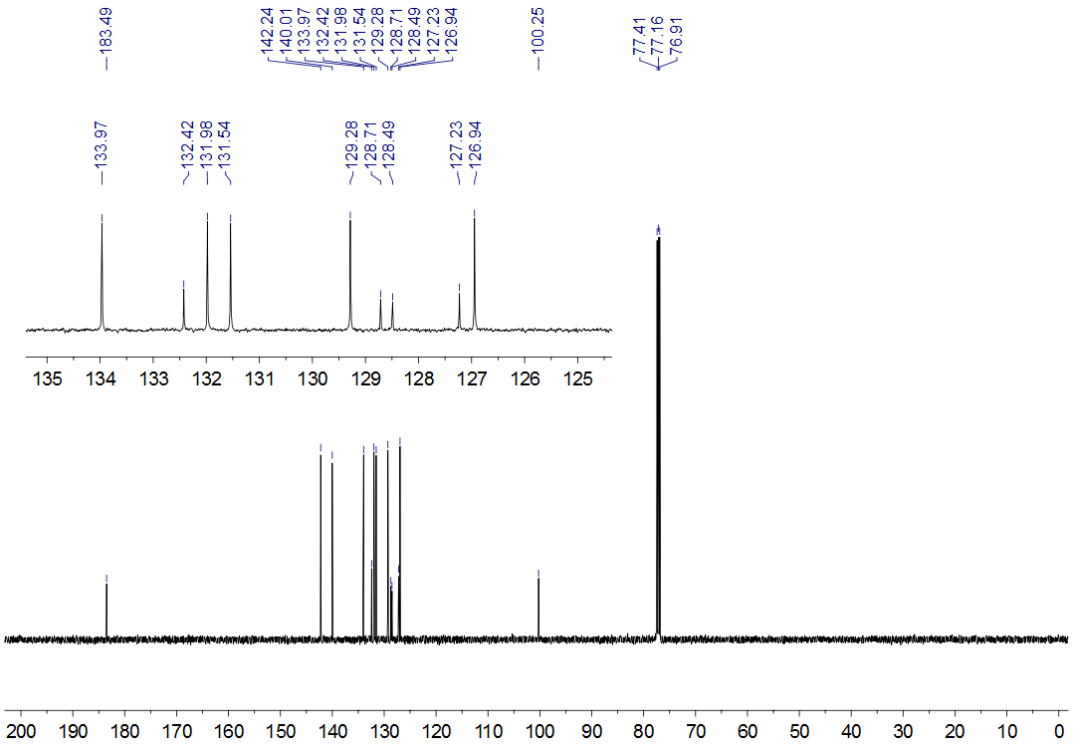


Figure 6 ^{13}C-NMR spectrum (125 MHz; $CDCl_3$) of 9-Iodo-1*H*-phenalen-1-one.

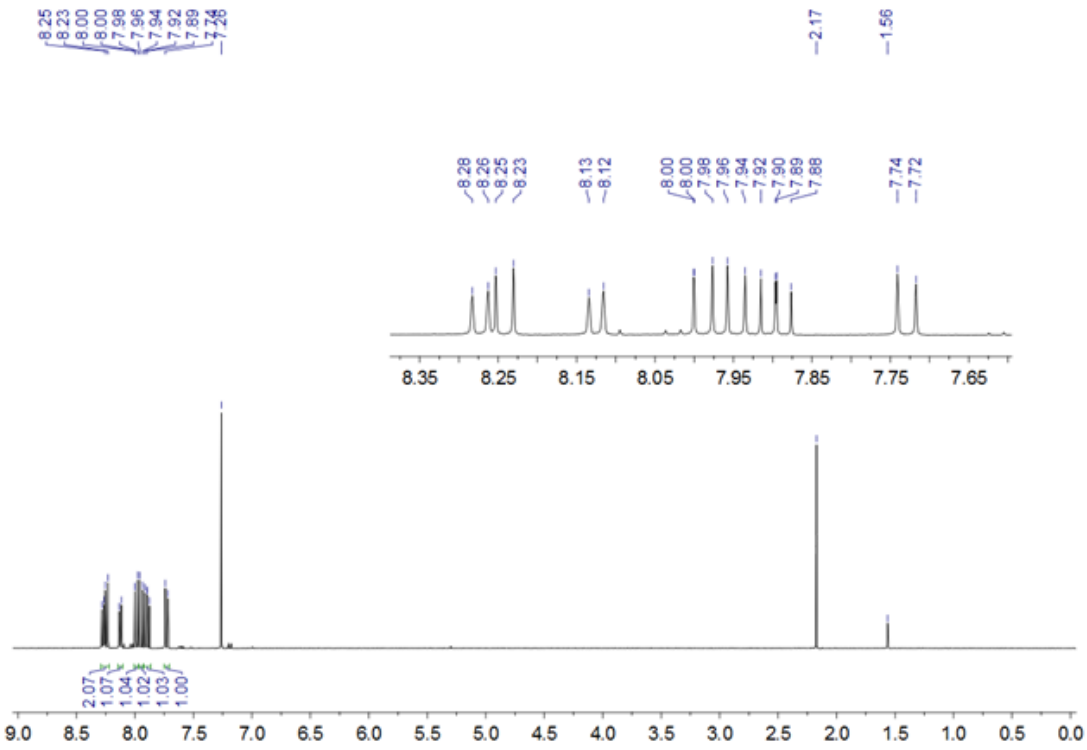


Figure 7 ^{1}H-NMR spectrum (400 MHz; $CDCl_3$) of phenaleno[1,9-*cd*]isoxazole.

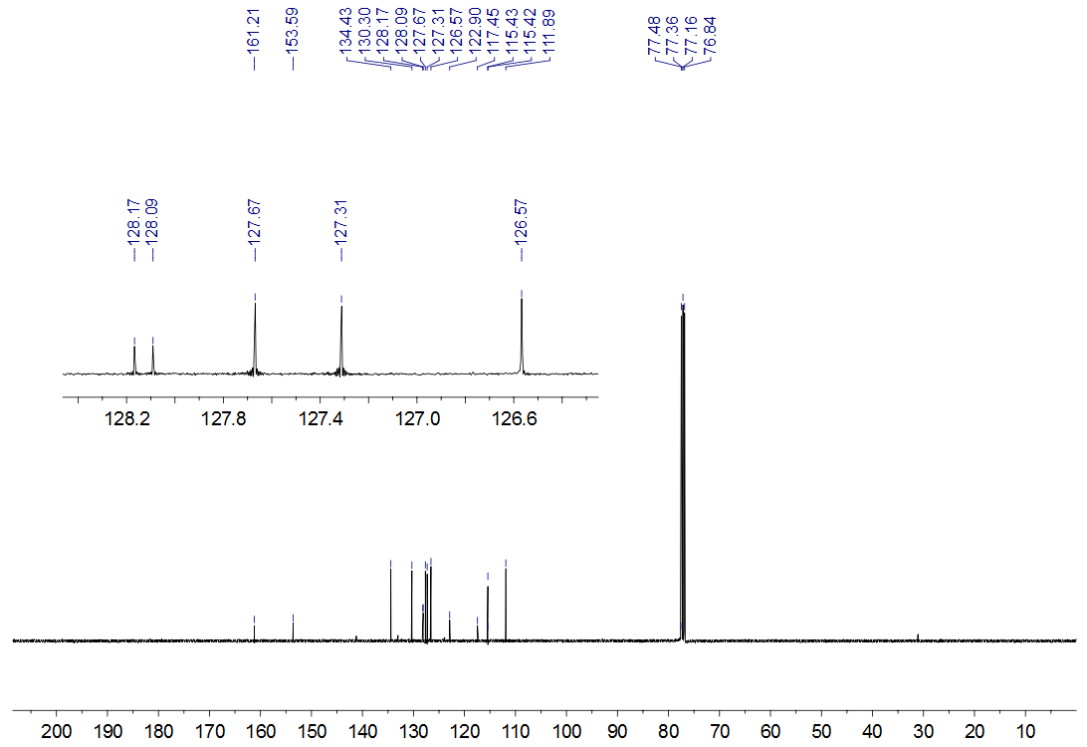


Figure 8 ^{13}C-NMR spectrum (100 MHz; $CDCl_3$) of phenaleno[1,9-*cd*]isoxazole.

X-ray diffraction data were collected at 150 K on an Oxford Diffraction Gemini A Ultra (Atlas CCD detector) or Bruker Apex II (Quasar CCD detector) diffractometer equipped with a graphite monochromated Mo Kα radiation (λ = 0.71073 Å) sources. Data reductions were carried out and absorption corrections applied using CrysAlisPro or Apex2 software [details in CIF]. The structures were all solved by direct methods using the program SHELXS97 and refined using full-matrix least-squares refinement on F^2 [SHELX Sheldrick, G. M. *Acta Cryst.* 2008, *A64*, 112-122] within the WinGX program suite [Farrugia, L. J. *J. Appl. Cryst.* 1999, *32*, 837-838].

Full refinement details are given in the CIF files. Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre (CCDC 943186-943189 contain the crystal structure data for compound 2, 3, 4 and 6), and copies of these data can be obtained free of charge via www. ccdc.cam.ac.uk/data_request/cif.

X-Ray structura analysis

Inter- and intramolecular separations between fluorine atoms and hydrogen atoms in compound **2** (Figure **9**).

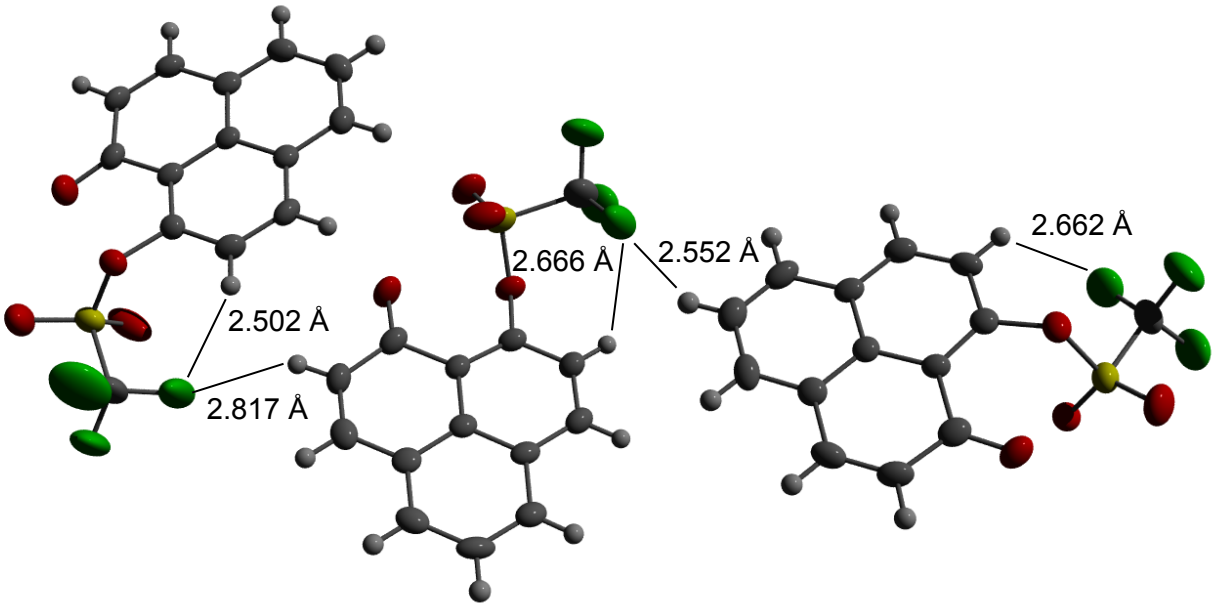
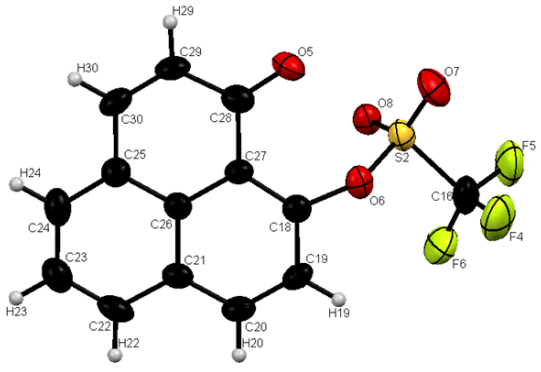


Figure 9

Crystal data and structure refinement for **1-oxo-1*H*-phenalen-9-yl trifluoromethanesulfonate**	
Empirical formula	$C_{14}H_7F_3O_4S$
Formula weight	328.26
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, Cc
Unit cell dimensions	a = 13.4040(4) A α = 90.00 deg. B = 25.1954(6) A β = 101.642(3) deg. C = 12.1027(4) A γ = 90.00 deg.
Volume	4003.23 A^3
Z, Calculated density	12, 1.634 Mg/m^3
Absorption coefficient	0.294 mm^-1
F(000)	1992
Crystal size	0.30 x 0.09 x 0.07 mm
Theta range for data collection	2.88 to 25.70 deg.
Limiting indices	-15<=h<=16, -30<=k<=30, -14<=l<=14
Reflections collected / unique	16213 / 6944 [R(int) = 0.0392]
Completeness to theta = 25.70	99.6 %
Absorption correction	Analytical
Max. and min. Transmission	0.9797 and 0.9169
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6944 / 2 / 596
Goodness-of-fit on F^{2}	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0417, wR2 = 0.0780
R indices (all data)	R1 = 0.0596, wR2 = 0.0876
Absolute structure parameter	-0.05(6)
Extinction coefficient	0.00033(8)
Largest diff. Peak and hole	0.24 and -0.24 e.A^-3

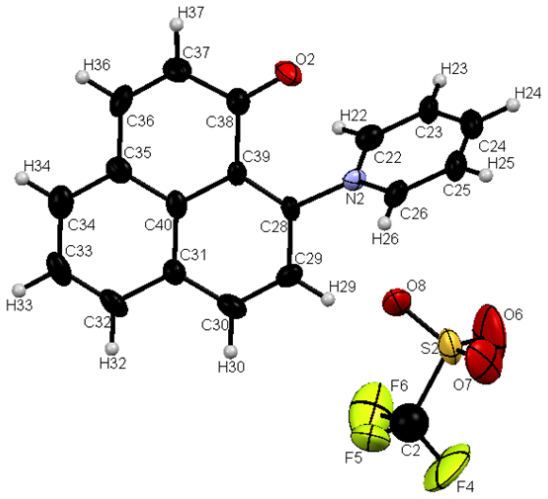


Bond Lengths			Bond angles			
Atom 1	Atom 2	Length	Atom 1	Atom 2	Atom 3	Angle
C16	F4	1.314(6)	F1	C1	F2	109.0(4)
C16	F5	1.335(5)	F1	C1	F3	110.6(4)
C16	F6	1.316(5)	F1	C1	S1	109.9(3)
C16	S2	1.828(4)	F2	C1	F3	109.1(4)
C18	C19	1.400(4)	F2	C1	S1	107.8(3)
C18	C27	1.382(4)	F3	C1	S1	110.4(3)
C18	O6	1.421(4)	C4	C3	C12	123.2(3)
C19	H19	0.951(3)	C4	C3	O2	115.7(3)
C19	C20	1.367(5)	C12	C3	O2	120.9(3)
C20	H20	0.951(3)	C3	C4	H4	120.5(3)
C20	C21	1.401(4)	C3	C4	C5	119.2(3)
C21	C22	1.418(5)	H4	C4	C5	120.3(3)
C21	C26	1.433(4)	C4	C5	H5	119.5(3)
C22	H22	0.951(3)	C4	C5	C6	121.1(3)
C22	C23	1.364(5)	H5	C5	C6	119.4(3)
C23	H23	0.951(4)	C5	C6	C7	121.6(3)
C23	C24	1.394(5)	C5	C6	C11	119.0(3)
C24	H24	0.951(3)	C7	C6	C11	119.3(3)
C24	C25	1.372(4)	C6	C7	H7	119.7(3)
C25	C26	1.424(4)	C6	C7	C8	120.7(3)
C25	C30	1.447(4)	H7	C7	C8	119.6(4)
C26	C27	1.424(4)	C7	C8	H8	120.0(4)
C27	C28	1.495(4)	C7	C8	C9	120.1(3)
C28	C29	1.455(5)	H8	C8	C9	119.9(4)
C28	O5	1.222(4)	C8	C9	H9	119.0(4)
C29	H29	0.950(3)	C8	C9	C10	121.8(3)
C29	C30	1.342(5)	H9	C9	C10	119.2(3)
C30	H30	0.949(3)	C9	C10	C11	119.0(3)
O6	S2	1.568(2)	C9	C10	C15	122.1(3)
O7	S2	1.409(2)	C11	C10	C15	118.9(3)
O8	S2	1.412(3)	C6	C11	C10	119.1(3)
			C6	C11	C12	120.4(3)
			C10	C11	C12	120.5(3)
			C3	C12	C11	117.0(3)
			C3	C12	C13	123.5(3)
			C11	C12	C13	119.5(3)
			C12	C13	C14	116.4(3)
			C12	C13	O1	121.9(3)
			C14	C13	O1	121.7(3)
			C13	C14	H14	118.5(3)
			C13	C14	C15	123.0(3)
			H14	C14	C15	118.5(3)
			C10	C15	C14	121.5(3)
			C10	C15	H15	119.2(3)
			C14	C15	H15	119.3(3)
			C3	O2	S1	122.6(2)
			C1	S1	O2	98.6(2)
			C1	S1	O3	106.5(2)
			C1	S1	O4	104.7(2)
			O2	S1	O3	111.3(1)
			O2	S1	O4	108.5(2)
			O3	S1	O4	124.0(2)

F4	C16	F5	108.1(3)
F4	C16	F6	109.6(3)
F4	C16	S2	111.3(3)
F5	C16	F6	108.4(3)
F5	C16	S2	107.7(3)
F6	C16	S2	111.6(3)
C19	C18	C27	123.0(3)
C19	C18	O6	114.8(3)
C27	C18	O6	121.9(3)
C18	C19	H19	120.3(3)
C18	C19	C20	119.4(3)
H19	C19	C20	120.4(3)
C19	C20	H20	119.4(3)
C19	C20	C21	121.3(3)
H20	C20	C21	119.3(3)
C20	C21	C22	122.6(3)
C20	C21	C26	118.6(3)
C22	C21	C26	118.7(3)
C21	C22	H22	119.5(3)
C21	C22	C23	121.0(3)
H22	C22	C23	119.5(4)
C22	C23	H23	119.9(4)
C22	C23	C24	120.2(3)
H23	C23	C24	119.9(4)
C23	C24	H24	119.1(4)
C23	C24	C25	121.7(3)
H24	C24	C25	119.2(3)
C24	C25	C26	119.7(3)
C24	C25	C30	121.2(3)
C26	C25	C30	119.1(3)
C21	C26	C25	118.8(3)
C21	C26	C27	120.4(3)
C25	C26	C27	120.9(3)
C18	C27	C26	117.2(3)
C18	C27	C28	123.5(3)
C26	C27	C28	119.3(3)
C27	C28	C29	116.4(3)
C27	C28	O5	122.3(3)
C29	C28	O5	121.2(3)
C28	C29	H29	118.6(3)
C28	C29	C30	123.0(3)
H29	C29	C30	118.5(4)
C25	C30	C29	121.4(3)
C25	C30	H30	119.3(3)
C29	C30	H30	119.3(3)
C18	O6	S2	123.3(2)
C16	S2	O6	98.1(2)
C16	S2	O7	105.7(2)
C16	S2	O8	106.1(2)
O6	S2	O7	108.8(1)
O6	S2	O8	111.4(1)
O7	S2	O8	123.4(1)
F7	C31	F8	108.9(4)
F7	C31	F9	109.7(4)

F7	C31	S3	110.1(3)
F8	C31	F9	109.5(4)
F8	C31	S3	108.0(3)
F9	C31	S3	110.6(3)
C34	C33	C42	123.8(3)
C34	C33	O10	114.8(3)
C42	C33	O10	121.1(3)
C33	C34	H34	120.6(3)
C33	C34	C35	118.9(3)
H34	C34	C35	120.5(3)
C34	C35	H35	119.6(3)
C34	C35	C36	120.9(3)
H35	C35	C36	119.5(3)
C35	C36	C37	121.6(3)
C35	C36	C41	119.3(3)
C37	C36	C41	119.1(3)
C36	C37	H37	119.7(3)
C36	C37	C38	120.7(3)
H37	C37	C38	119.7(3)
C37	C38	H38	119.8(3)
C37	C38	C39	120.4(3)
H38	C38	C39	119.8(3)
C38	C39	H39	119.5(3)
C38	C39	C40	120.9(3)
H39	C39	C40	119.6(3)
C39	C40	C41	119.7(3)
C39	C40	C45	121.5(3)
C41	C40	C45	118.7(3)
C36	C41	C40	119.2(3)
C36	C41	C42	119.9(3)
C40	C41	C42	120.9(3)
C33	C42	C41	117.3(3)
C33	C42	C43	123.6(3)
C41	C42	C43	119.0(3)
C42	C43	C44	116.4(3)
C42	C43	O9	121.9(3)
C44	C43	O9	121.7(3)
C43	C44	H44	118.9(3)
C43	C44	C45	122.4(3)
H44	C44	C45	118.8(4)
C40	C45	C44	122.5(3)
C40	C45	H45	118.8(3)
C44	C45	H45	118.7(4)
C33	O10	S3	122.1(2)
C31	S3	O10	98.4(2)
C31	S3	O11	106.6(2)
C31	S3	O12	105.0(2)
O10	S3	O11	111.7(1)
O10	S3	O12	108.5(1)
O11	S3	O12	123.5(2)

Crystal data and structure refinement for **1-(1-oxo-1*H*-phenalen-9-yl)pyridinium triflate**	
Empirical formula	$C_{20.50}H_{15}F_3NO_{4.50}S$
Formula weight	436.4
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P 2_1 2_1 2_1
Unit cell dimensions	a = 23.961(5) A α = 90 deg. B = 23.211(5) A β = 90 deg. C = 6.8908(16) A γ = 90 deg.
Volume	3832.38 A^3
Z, Calculated density	8, 1.513 Mg/m^3
Absorption coefficient	0.229 mm^-1
F(000)	1792
Crystal size	0.13 x 0.10 x 0.06 mm
Theta range for data collection	1.95 to 25.43 deg.
Limiting indices	-23<=h<=28, -28<=k<=24, -8<=l<=7
Reflections collected / unique	23837 / 6873 [R(int) = 0.1786]
Completeness to theta = 25.43	99.5 %
Absorption correction	Empirical
Max. and min. Transmission	0.9864 and 0.9708
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6873 / 0 / 540
Goodness-of-fit on F^{2}	0.997
Final R indices [I>2sigma(I)]	R1 = 0.0736, wR2 = 0.1198
R indices (all data)	R1 = 0.2125, wR2 = 0.1668
Absolute structure parameter	0.17(17)
Extinction coefficient	0.0019(3)
Largest diff. Peak and hole	0.36 and -0.35 e.A^-3

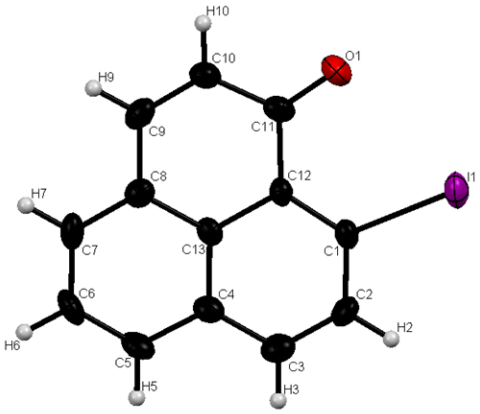


Bond lengths			Bond angles			
Atom 1	Atom 2	Length	Atom 1	Atom 2	Atom 3	Angle
C2	F4	1.24(1)	F1	C1	F2	108.3(8)
C2	F5	1.34(1)	F1	C1	F3	106.4(7)
C2	F6	1.34(2)	F1	C1	S1	109.5(6)
C2	S2	1.85(1)	F2	C1	F3	108.9(8)
O6	S2	1.427(8)	F2	C1	S1	113.3(7)
O7	S2	1.424(7)	F3	C1	S1	110.3(6)
O8	S2	1.447(5)	C1	S1	O3	103.0(4)
C22	H22	0.950(8)	C1	S1	O4	102.3(4)
C22	C23	1.37(1)	C1	S1	O5	104.1(4)
C22	N2	1.36(1)	O3	S1	O4	114.2(3)
C23	H23	0.951(8)	O3	S1	O5	115.5(3)
C23	C24	1.37(1)	O4	S1	O5	115.2(3)
C24	H24	0.949(7)	F4	C2	F5	110.2(9)
C24	C25	1.36(1)	F4	C2	F6	111(1)
C25	H25	0.951(9)	F4	C2	S2	113.5(8)
C25	C26	1.38(1)	F5	C2	F6	105.8(9)
C26	H26	0.949(8)	F5	C2	S2	107.6(7)
C26	N2	1.33(1)	F6	C2	S2	108.8(8)
C28	C29	1.407(9)	C2	S2	O6	101.5(5)
C28	C39	1.35(1)	C2	S2	O7	103.5(5)
C28	N2	1.462(7)	C2	S2	O8	102.7(4)
C29	H29	0.951(7)	O6	S2	O7	115.1(4)
C29	C30	1.36(1)	O6	S2	O8	115.6(4)
C30	H30	0.950(7)	O7	S2	O8	115.5(4)
C30	C31	1.40(1)	H3	C3	C4	119.4(7)
C31	C32	1.42(1)	H3	C3	N1	119.4(7)
C31	C40	1.41(1)	C4	C3	N1	121.2(7)
C32	H32	0.951(7)	C3	C4	H4	120.2(8)
C32	C33	1.34(1)	C3	C4	C5	119.6(7)
C33	H33	0.950(7)	H4	C4	C5	120.2(8)
C33	C34	1.40(1)	C4	C5	H5	120.5(8)
C34	H34	0.950(7)	C4	C5	C6	118.8(7)
C34	C35	1.38(1)	H5	C5	C6	120.6(7)
C35	C36	1.46(1)	C5	C6	H6	120.3(7)
C35	C40	1.40(1)	C5	C6	C7	119.2(7)
C36	H36	0.949(7)	H6	C6	C7	120.5(7)
C36	C37	1.34(1)	C6	C7	H7	119.6(7)
C37	H37	0.950(7)	C6	C7	N1	120.6(7)
C37	C38	1.43(1)	H7	C7	N1	119.8(7)
C38	C39	1.52(1)	C10	C9	C20	123.7(7)
C38	O2	1.227(9)	C10	C9	N1	113.8(6)
C39	C40	1.42(1)	C20	C9	N1	122.4(7)
			C9	C10	H10	121.4(7)
			C9	C10	C11	117.2(7)
			H10	C10	C11	121.4(7)
			C10	C11	H11	118.7(7)
			C10	C11	C12	122.7(7)
			H11	C11	C12	118.6(7)
			C11	C12	C13	123.3(7)
			C11	C12	C21	118.1(7)
			C13	C12	C21	118.5(6)
			C12	C13	H13	119.3(7)

C12	C13	C14	121.5(7)
H13	C13	C14	119.3(7)
C13	C14	H14	119.9(8)
C13	C14	C15	120.4(7)
H14	C14	C15	119.7(8)
C14	C15	H15	119.5(7)
C14	C15	C16	121.1(7)
H15	C15	C16	119.4(7)
C15	C16	C17	121.9(7)
C15	C16	C21	119.7(7)
C17	C16	C21	118.3(6)
C16	C17	H17	119.2(7)
C16	C17	C18	121.6(7)
H17	C17	C18	119.2(7)
C17	C18	H18	118.2(7)
C17	C18	C19	123.6(7)
H18	C18	C19	118.2(7)
C18	C19	C20	115.1(6)
C18	C19	O1	122.1(7)
C20	C19	O1	122.7(7)
C9	C20	C19	123.0(7)
C9	C20	C21	118.4(7)
C19	C20	C21	118.5(6)
C12	C21	C16	118.7(6)
C12	C21	C20	119.6(7)
C16	C21	C20	121.6(7)
C3	N1	C7	120.5(6)
C3	N1	C9	119.5(6)
C7	N1	C9	120.0(6)
H22	C22	C23	120.0(8)
H22	C22	N2	119.8(7)
C23	C22	N2	120.1(7)
C22	C23	H23	120.6(8)
C22	C23	C24	118.7(7)
H23	C23	C24	120.7(8)
C23	C24	H24	119.5(8)
C23	C24	C25	120.9(8)
H24	C24	C25	119.6(8)
C24	C25	H25	120.4(8)
C24	C25	C26	118.9(7)
H25	C25	C26	120.7(8)
C25	C26	H26	119.9(8)
C25	C26	N2	120.2(7)
H26	C26	N2	119.9(7)
C29	C28	C39	122.7(6)
C29	C28	N2	115.0(6)
C39	C28	N2	122.3(6)
C28	C29	H29	120.8(7)
C28	C29	C30	118.6(7)
H29	C29	C30	120.5(7)
C29	C30	H30	119.4(7)
C29	C30	C31	121.4(7)
H30	C30	C31	119.2(7)
C30	C31	C32	122.2(7)

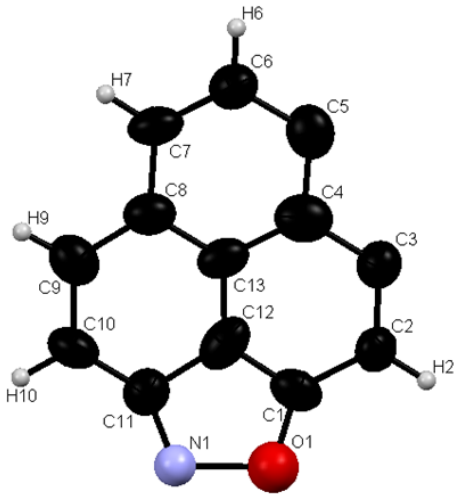
C30	C31	C40	119.1(7)
C32	C31	C40	118.7(7)
C31	C32	H32	119.5(7)
C31	C32	C33	120.9(7)
H32	C32	C33	119.5(8)
C32	C33	H33	119.7(8)
C32	C33	C34	120.7(7)
H33	C33	C34	119.6(8)
C33	C34	H34	120.0(7)
C33	C34	C35	120.2(7)
H34	C34	C35	119.9(7)
C34	C35	C36	120.5(7)
C34	C35	C40	120.2(7)
C36	C35	C40	119.2(7)
C35	C36	H36	119.7(7)
C35	C36	C37	120.9(7)
H36	C36	C37	119.4(7)
C36	C37	H37	118.4(7)
C36	C37	C38	123.5(7)
H37	C37	C38	118.2(7)
C37	C38	C39	116.2(6)
C37	C38	O2	121.9(7)
C39	C38	O2	121.7(7)
C28	C39	C38	122.9(6)
C28	C39	C40	118.8(7)
C38	C39	C40	118.3(6)
C31	C40	C35	119.2(7)
C31	C40	C39	119.3(7)
C35	C40	C39	121.5(7)
C22	N2	C26	121.2(6)
C22	N2	C28	118.8(6)
C26	N2	C28	119.9(6)
H41A	C41	H41B	109.5(8)
H41A	C41	H41C	109.4(8)
H41A	C41	C42	109.5(8)
H41B	C41	H41C	109.5(8)
H41B	C41	C42	109.5(8)
H41C	C41	C42	109.5(8)
C41	C42	C43	117.2(7)
C41	C42	O9	121.3(8)
C43	C42	O9	121.5(8)
C42	C43	H43A	109.4(8)
C42	C43	H43B	109.5(8)
C42	C43	H43C	109.4(8)
H43A	C43	H43B	109.4(8)
H43A	C43	H43C	109.5(8)
H43B	C43	H43C	109.5(8)

Crystal data and structure refinement for **9-iodo-1*H*-phenalen-1-one**	
Empirical formula	$C_{13}H_7IO$
Formula weight	306.09
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 12.8997(18) A α = 90 deg. B = 12.184(2) A β = 101.649(10)deg. C = 13.1411(13) A γ = 90 deg.
Volume	2022.9(5) A^3
Z, Calculated density	8, 2.010 Mg/m^3
Absorption coefficient	3.131 mm^-1
F(000)	1168
Crystal size	0.18 x 0.10 x 0.08 mm
Theta range for data collection	2.99 to 25.47 deg.
Limiting indices	-15<=h<=15, -14<=k<=14, -15<=l<=15
Reflections collected / unique	8018 / 1872 [R(int) = 0.0399]
Completeness to theta = 25.47	99.4 %
Absorption correction	Analytical
Max. and min. Transmission	0.7878 and 0.6026
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1872 / 0 / 136
Goodness-of-fit on F^2	1.122
Final R indices [I>2sigma(I)]	R1 = 0.0338, wR2 = 0.0652
R indices (all data)	R1 = 0.0464, wR2 = 0.0712
Extinction coefficient	none
Largest diff. Peak and hole	0.53 and -0.56 e.A^-3



Bond lengths			Bond angles			
Atom 1	Atom 2	Length	Atom1	Atom2	Atom3	Angle
C1	C2	1.395(7)	C2	C1	C12	121.8(4)
C1	C12	1.387(6)	C2	C1	I1	114.3(3)
C1	I1	2.111(4)	C12	C1	I1	123.8(3)
C2	H2	0.950(5)	C1	C2	H2	119.4(4)
C2	C3	1.365(7)	C1	C2	C3	121.1(4)
C3	H3	0.949(5)	H2	C2	C3	119.5(5)
C3	C4	1.410(7)	C2	C3	H3	119.7(5)
C4	C5	1.419(7)	C2	C3	C4	120.6(4)
C4	C13	1.410(7)	H3	C3	C4	119.7(5)
C5	H5	0.950(5)	C3	C4	C5	122.2(4)
C5	C6	1.372(7)	C3	C4	C13	118.9(4)
C6	H6	0.949(5)	C5	C4	C13	118.9(4)
C6	C7	1.391(8)	C4	C5	H5	119.4(5)
C7	H7	0.951(4)	C4	C5	C6	121.2(5)
C7	C8	1.381(6)	H5	C5	C6	119.4(5)
C8	C9	1.456(7)	C5	C6	H6	120.2(5)
C8	C13	1.425(6)	C5	C6	C7	119.8(5)
C9	H9	0.951(5)	H6	C6	C7	120.1(5)
C9	C10	1.340(7)	C6	C7	H7	119.4(5)
C10	H10	0.951(5)	C6	C7	C8	121.1(4)
C10	C11	1.453(7)	H7	C7	C8	119.4(4)
C11	C12	1.492(7)	C7	C8	C9	120.6(4)
C11	O1	1.221(7)	C7	C8	C13	120.0(4)
C12	C13	1.455(6)	C9	C8	C13	119.4(4)
			C8	C9	H9	119.5(5)
			C8	C9	C10	121.0(4)
			H9	C9	C10	119.5(5)
			C9	C10	H10	118.4(5)
			C9	C10	C11	123.4(4)
			H10	C10	C11	118.2(4)
			C10	C11	C12	117.0(4)
			C10	C11	O1	120.9(4)
			C12	C11	O1	122.1(4)
			C1	C12	C11	124.5(4)
			C1	C12	C13	117.1(4)
			C11	C12	C13	118.4(4)
			C4	C13	C8	119.0(4)
			C4	C13	C12	120.5(4)
			C8	C13	C12	120.5(4)

Crystal data and structure refinement for **Phenaleno[1,9-*cd*]isoxazole**	
Empirical formula	$C_{13}H_7N\ O$
Formula weight	193.20
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 7.5727(9) A α = 100.949(10) deg. B = 8.2341(9) A β = 96.440(10) deg. C = 14.4327(19) A γ = 94.028(9) deg.
Volume	874.11(18) A^3
Z, Calculated density	4, 1.468 Mg/m^3
Absorption coefficient	0.094 mm^-1
F(000)	400
Crystal size	0.28 x 0.23 x 0.21 mm
Theta range for data collection	2.72 to 24.47 deg.
Limiting indices	-8<=h<=8, -9<=k<=9, -16<=l<=16
Reflections collected / unique	8715 / 4372 [R(int) = 0.105]
Completeness to theta = 24.47	99.3 %
Absorption correction	Empirical
Max. and min. Transmission	1.000 and 0.757
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4372 / 16 / 270
Goodness-of-fit on F^2	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0976, wR2 = 0.2800
R indices (all data)	R1 = 0.1768, wR2 = 0.3178
Extinction coefficient	none
Largest diff. Peak and hole	0.75 and -0.22 e.A^-3



Bond lengths			Bond angles			
Atom 1	Atom 2	Length	Atom 1	Atom 2	Atom 3	Angle
C1	C2	1.407(9)	C2	C1	C12	119.0(6)
C1	C12	1.368(9)	C2	C1	O1	133.0(7)
C1	O1	1.28(1)	C12	C1	O1	108.0(6)
C2	H2	0.950(6)	C1	C2	H2	120.6(6)
C2	C3	1.364(9)	C1	C2	C3	118.7(6)
C3	C4	1.421(9)	H2	C2	C3	120.7(6)
C4	C5	1.400(9)	C2	C3	C4	120.7(6)
C4	C13	1.413(9)	C3	C4	C5	118.7(6)
C5	C6	1.427(9)	C3	C4	C13	121.2(6)
C6	H6	0.950(7)	C5	C4	C13	120.1(6)
C6	C7	1.373(9)	C4	C5	C6	117.6(6)
C7	H7	0.949(6)	C5	C6	H6	119.0(6)
C7	C8	1.418(8)	C5	C6	C7	121.9(6)
C8	C9	1.393(9)	H6	C6	C7	119.1(6)
C8	C13	1.380(9)	C6	C7	H7	120.0(6)
C9	H9	0.950(7)	C6	C7	C8	120.0(6)
C9	C10	1.419(9)	H7	C7	C8	120.0(6)
C10	H10	0.950(6)	C7	C8	C9	124.5(6)
C10	C11	1.373(9)	C7	C8	C13	118.8(6)
C11	C12	1.451(9)	C9	C8	C13	116.7(6)
C11	N1	1.26(1)	C8	C9	H9	119.4(6)
C12	C13	1.368(9)	C8	C9	C10	121.2(6)
N1	O1	1.55(1)	H9	C9	C10	119.4(6)
			C9	C10	H10	119.0(6)
			C9	C10	C11	122.1(6)
			H10	C10	C11	119.0(6)
			C10	C11	C12	115.9(6)
			C10	C11	N1	143.0(7)
			C12	C11	N1	100.8(6)
			C1	C12	C11	113.9(6)
			C1	C12	C13	125.6(6)
			C11	C12	C13	120.5(6)
			C4	C13	C8	121.5(6)
			C4	C13	C12	114.9(6)
			C8	C13	C12	123.6(6)
			C11	N1	O1	113.1(8)
			C1	O1	N1	104.2(7)
			C15	C14	C25	119.3(7)
			C15	C14	O2	135.8(8)
			C25	C14	O2	104.8(7)
			C14	C15	H15	120.7(7)
			C14	C15	C16	118.5(7)
			H15	C15	C16	120.7(7)
			C15	C16	C17	123.5(7)
			C16	C17	C18	121.6(8)
			C16	C17	C26	118.5(8)
			C18	C17	C26	119.9(8)
			C17	C18	C19	117.9(7)
			C18	C19	H19	119.3(8)
			C18	C19	C20	121.2(7)
			H19	C19	C20	119.5(7)
			C19	C20	H20	118.7(7)

C19	C20	C21	122.6(7)
H20	C20	C21	118.7(8)
C20	C21	C22	125.8(7)
C20	C21	C26	117.0(7)
C22	C21	C26	117.2(6)
C21	C22	H22	120.2(7)
C21	C22	C23	119.6(7)
H22	C22	C23	120.2(7)
C22	C23	H23	118.7(9)
C22	C23	C24	122.7(8)
H23	C23	C24	118.7(9)
C23	C24	C25	113.0(8)
C23	C24	N2	136.8(9)
C25	C24	N2	110.2(9)
C14	C25	C24	110.9(7)
C14	C25	C26	116.9(7)
C24	C25	C26	132.1(8)
C17	C26	C21	121.5(7)
C17	C26	C25	123.1(7)
C21	C26	C25	115.4(6)
C24	N2	O2	105.7(8)
C14	O2	N2	108.3(8)

Calculated geometry (AM1) of 9-iodophenalenone 4

C	0.623000000	-0.129000000	1.260000000
C	-2.024000000	0.846000000	1.086000000
C	-0.021000000	-0.020000000	-0.018000000
C	-0.038000000	0.327000000	2.386000000
C	-1.370000000	0.807000000	2.289000000
C	-1.358000000	0.443000000	-0.102000000
H	-1.886000000	1.147000000	3.202000000
H	-3.065000000	1.199000000	1.020000000
C	-2.008000000	0.513000000	-1.363000000
H	-3.053000000	0.856000000	-1.399000000
C	-1.341000000	0.161000000	-2.512000000
H	-1.842000000	0.210000000	-3.490000000
C	0.004000000	-0.260000000	-2.448000000
H	0.531000000	-0.515000000	-3.381000000
C	0.659000000	-0.347000000	-1.233000000
C	1.967000000	-0.764000000	1.296000000
C	2.673000000	-0.905000000	0.011000000
H	3.733000000	-1.194000000	0.083000000
C	2.053000000	-0.737000000	-1.167000000
H	2.581000000	-0.883000000	-2.123000000
O	2.482000000	-1.211000000	2.329000000
I	0.701000000	0.456000000	4.274000000

Heat of Formation: 220.975 kJ/mol

Calculated geometry (M05-2X/SDD) of 9-iodophenalenone 4

C	0.353926000	0.368532000	-0.000002000
C	0.964629000	-2.406804000	0.000004000
C	1.722801000	-0.077662000	-0.000001000
C	-0.658504000	-0.593023000	-0.000006000
C	-0.345517000	-1.981126000	0.000005000
C	2.030144000	-1.467232000	-0.000001000
H	-1.151076000	-2.702230000	0.000006000
H	1.190857000	-3.466621000	0.000004000

C	3.386580000	-1.900906000	-0.000002000
H	3.593978000	-2.964679000	-0.000003000
C	4.418534000	-0.981367000	-0.000002000
H	5.448840000	-1.311719000	-0.000001000
C	4.121182000	0.402879000	-0.000002000
H	4.929247000	1.125534000	-0.000001000
C	2.807065000	0.856484000	0.000001000
C	0.085130000	1.840126000	-0.000004000
C	1.247314000	2.744000000	0.000008000
H	1.009740000	3.799844000	0.000023000
C	2.517414000	2.283000000	0.000002000
H	3.355541000	2.971081000	0.000010000
O	-1.071532000	2.324852000	-0.000008000
I	-2.749227000	-0.199461000	0.000001000

E(RM052X) = -586.060888383

Number of vibrational modes with imaginary frequency: 0

Calculated geometry (M06/SDD) of 9-iodophenalenone 4

C	0.000000000	0.512537000	0.000000000
C	2.361780000	-1.075252000	0.000000000
C	1.298211000	1.132865000	0.000000000
C	-0.064895000	-0.887277000	0.000000000
C	1.118397000	-1.674087000	0.000000000
C	2.483432000	0.338724000	0.000000000
H	1.034544000	-2.756123000	0.000000000
H	3.261666000	-1.685305000	0.000000000
C	3.762217000	0.961914000	0.000000000
H	4.648773000	0.332340000	0.000000000
C	3.875369000	2.342002000	0.000000000
H	4.851685000	2.814731000	0.000000000
C	2.707108000	3.136290000	0.000000000
H	2.790211000	4.220768000	0.000000000
C	1.438415000	2.557296000	0.000000000

C	-1.211810000	1.389833000	0.000000000
C	-0.990129000	2.841920000	0.000000000
H	-1.892911000	3.444747000	0.000000000
C	0.250532000	3.386696000	0.000000000
H	0.384705000	4.466507000	0.000000000
O	-2.384855000	0.941016000	0.000000000
I	-1.852294000	-2.040501000	0.000000000

E(RM06) = -585.716982237

Number of vibrational modes with imaginary frequency: 0

Calculated geometry (M06/6-31+G(d,p), pcm, DMF) of triflate 2

6	1.001794000	0.269406000	-0.292196000
6	1.981926000	-2.392823000	-0.335508000
6	2.388933000	0.005320000	-0.100697000
6	0.180417000	-0.826004000	-0.514824000
6	0.644409000	-2.145955000	-0.538252000
6	2.882083000	-1.327858000	-0.115873000
1	-0.066300000	-2.946437000	-0.725944000
1	2.358793000	-3.412917000	-0.350405000
6	4.266433000	-1.564846000	0.084779000
1	4.625956000	-2.591601000	0.071011000
6	5.134338000	-0.519414000	0.290786000
1	6.193180000	-0.706409000	0.444234000
6	4.649236000	0.801081000	0.300821000
1	5.338017000	1.628423000	0.460823000
6	3.304067000	1.074737000	0.110716000
6	0.497224000	1.665780000	-0.246777000
6	1.496341000	2.709392000	-0.053704000
1	1.123404000	3.730250000	-0.039588000
6	2.805388000	2.428130000	0.119132000
1	3.525171000	3.230622000	0.274734000
8	-0.700469000	1.944500000	-0.356456000
8	-1.178836000	-0.652159000	-0.793535000
16	-2.227388000	-0.827571000	0.421132000

8	-2.880622000	-2.110075000	0.271683000
8	-1.621897000	-0.432188000	1.672527000
6	-3.496035000	0.475670000	-0.083098000
9	-4.683671000	-0.030488000	0.210863000
9	-3.308953000	1.574364000	0.610395000
9	-3.432348000	0.722002000	-1.374433000

E(RM06) = -1535.675779

Number of vibrational modes with imaginary frequency: 0

Calculated geometry (M06/6-31+G(d,p), pcm, DMF) of the transition state for reaction of triflate 2 with azide anion

1	4.556507000	-1.902121000	1.617716000
6	3.963152000	-1.019174000	1.383305000
6	2.768083000	-1.184292000	0.676094000
6	3.626280000	1.356043000	1.472892000
6	1.968903000	-0.052775000	0.352495000
6	4.397672000	0.242366000	1.782098000
6	2.422131000	1.229372000	0.768123000
6	0.739385000	-0.210350000	-0.359557000
1	5.330020000	0.354200000	2.328978000
1	1.951168000	3.352900000	0.786822000
1	3.950955000	2.350562000	1.776148000
6	0.003070000	0.962009000	-0.693498000
6	0.442749000	2.244318000	-0.205570000
1	-0.184155000	3.103363000	-0.433393000
6	1.615509000	2.370824000	0.457557000
6	0.334822000	-1.524279000	-0.845672000
6	1.184119000	-2.644327000	-0.458146000
1	0.857856000	-3.628071000	-0.789993000
6	2.323934000	-2.481414000	0.254438000
1	2.939036000	-3.342773000	0.515414000
8	-0.671911000	-1.716350000	-1.558188000
8	-1.443638000	0.858742000	-0.789750000
16	-2.357730000	0.898716000	0.508531000
8	-1.619414000	1.210907000	1.714309000

8 -3.560988000 1.614496000 0.142245000

6 -2.897485000 -0.875390000 0.683848000

9 -3.403779000 -1.318861000 -0.448027000

9 -1.896002000 -1.637205000 1.077886000

9 -3.840746000 -0.884353000 1.620767000

7 1.964088000 0.019594000 -3.270433000

7 1.036769000 0.656178000 -2.978135000

7 0.084957000 1.277989000 -2.590460000

E(RM06) = -1699.9128941

Number of vibrational modes with imaginary frequency: 1

Calculated geometry (M06/6-31+G(d,p), pcm, DMF) of azide anion

7 0.000000000 0.000000000 0.000000000

7 0.000000000 0.000000000 1.184050000

7 0.000000000 0.000000000 -1.184050000

E(RM06) = -164.2501695

Number of vibrational modes with imaginary frequency: 0

Calculated geometry (M06/cc-pVTZ, pcm, DMF) of azide 5

6 0.000000000 0.594607000 0.000000000

6 1.292267000 -1.909333000 0.000000000

6 -0.756031000 -0.608061000 0.000000000

6 1.391402000 0.495946000 0.000000000

6 2.023804000 -0.763437000 0.000000000

6 -0.114241000 -1.868421000 0.000000000

1 3.104491000 -0.816309000 0.000000000

1 1.789004000 -2.871985000 0.000000000

6 -0.879051000 -3.050085000 0.000000000

1 -0.359810000 -4.000789000 0.000000000

6 -2.246366000 -3.000553000 0.000000000

1 -2.829554000 -3.910914000 0.000000000

6 -2.889015000 -1.760503000 0.000000000

1 -3.971468000 -1.711779000 0.000000000

6 -2.173926000 -0.580367000 0.000000000

6	-0.705539000	1.894550000	0.000000000
6	-2.161455000	1.842358000	0.000000000
1	-2.662284000	2.802127000	0.000000000
6	-2.843201000	0.689485000	0.000000000
1	-3.927516000	0.688089000	0.000000000
8	-0.132353000	2.976908000	0.000000000
7	2.159183000	1.662153000	0.000000000
7	3.380463000	1.570951000	0.000000000
7	4.500937000	1.645349000	0.000000000

E(RM06) = -738.7577067

E(CCSD(RHF)/cc-pVTZ//M06/cc-pVTZ), COSMO, DMF: -737.582222038

E(CCSD(UHF)/cc-pVTZ//M06/cc-pVTZ), pcm, DMF: -737.5704544

Number of vibrational modes with imaginary frequency: 0

Calculated geometry (M06/cc-pVTZ, pcm, DMF) of the transition state for dediazotation of azide 5, leading to 6

6	0.231817000	0.492601000	-0.000102000
6	0.082420000	-2.273353000	0.000402000
6	-1.025363000	-0.128686000	0.000017000
6	1.437126000	-0.254374000	0.000031000
6	1.300112000	-1.679453000	0.000288000
6	-1.129038000	-1.533582000	0.000276000
1	2.196826000	-2.283811000	0.000393000
1	0.026180000	-3.355715000	0.000597000
6	-2.394055000	-2.125726000	0.000396000
1	-2.469239000	-3.206520000	0.000594000
6	-3.533797000	-1.346861000	0.000265000
1	-4.508965000	-1.814179000	0.000362000
6	-3.432884000	0.038880000	0.000008000
1	-4.329542000	0.647765000	-0.000091000
6	-2.194150000	0.667607000	-0.000119000
6	0.373836000	1.910442000	-0.000351000
6	-0.838486000	2.694841000	-0.000491000
1	-0.740988000	3.772446000	-0.000683000
6	-2.046991000	2.091501000	-0.000379000

1	-2.950331000	2.691557000	-0.000484000
8	1.520858000	2.397161000	-0.000433000
7	2.581702000	0.446553000	-0.000093000
7	3.849975000	-0.671732000	0.000123000
7	4.943452000	-0.767942000	0.000159000

E(RM06) = -738.7102838

E(CCSD(RHF)/cc-pVTZ//M06/cc-pVTZ), COSMO, DMF: -737.543568535

E(CCSD(UHF)/cc-pVTZ//M06/cc-pVTZ), pcm, DMF: -737.5387023

Number of vibrational modes with imaginary frequency: 1

Calculated geometry (M06/6-31+G(d,p), pcm, DMF) of the transition state for reaction of triflate 2 with chloride anion

6	-1.199807000	0.421562000	0.405478000
6	-1.704224000	-2.368747000	0.581734000
6	-2.421742000	-0.124960000	-0.079400000
6	-0.218309000	-0.459181000	1.002859000
6	-0.538613000	-1.883905000	1.057560000
6	-2.700280000	-1.518512000	-0.002712000
1	0.206463000	-2.531612000	1.512174000
1	-1.907767000	-3.436538000	0.652450000
6	-3.909313000	-2.026670000	-0.479824000
1	-4.091178000	-3.098413000	-0.406785000
6	-4.872216000	-1.188084000	-1.039984000
1	-5.809851000	-1.596210000	-1.407722000
6	-4.617860000	0.175232000	-1.119081000
1	-5.359899000	0.846850000	-1.549891000
6	-3.414376000	0.722024000	-0.651480000
6	-0.931644000	1.832602000	0.293773000
6	-1.985260000	2.654186000	-0.280033000
1	-1.783619000	3.721827000	-0.346739000
6	-3.152253000	2.126600000	-0.728111000
1	-3.918196000	2.769493000	-1.162661000
8	0.159789000	2.342992000	0.648079000
16	2.221511000	0.555432000	-0.269911000
8	1.836055000	1.288079000	-1.464880000

8	2.931786000	1.221935000	0.807411000
6	3.433507000	-0.709042000	-0.892892000
9	4.484896000	-0.057055000	-1.383044000
9	3.842686000	-1.500269000	0.090011000
9	2.903811000	-1.449702000	-1.857138000
8	1.169625000	-0.506868000	0.177949000
17	0.391390000	0.047834000	2.683736000

E(RM06) = -1995.9821283

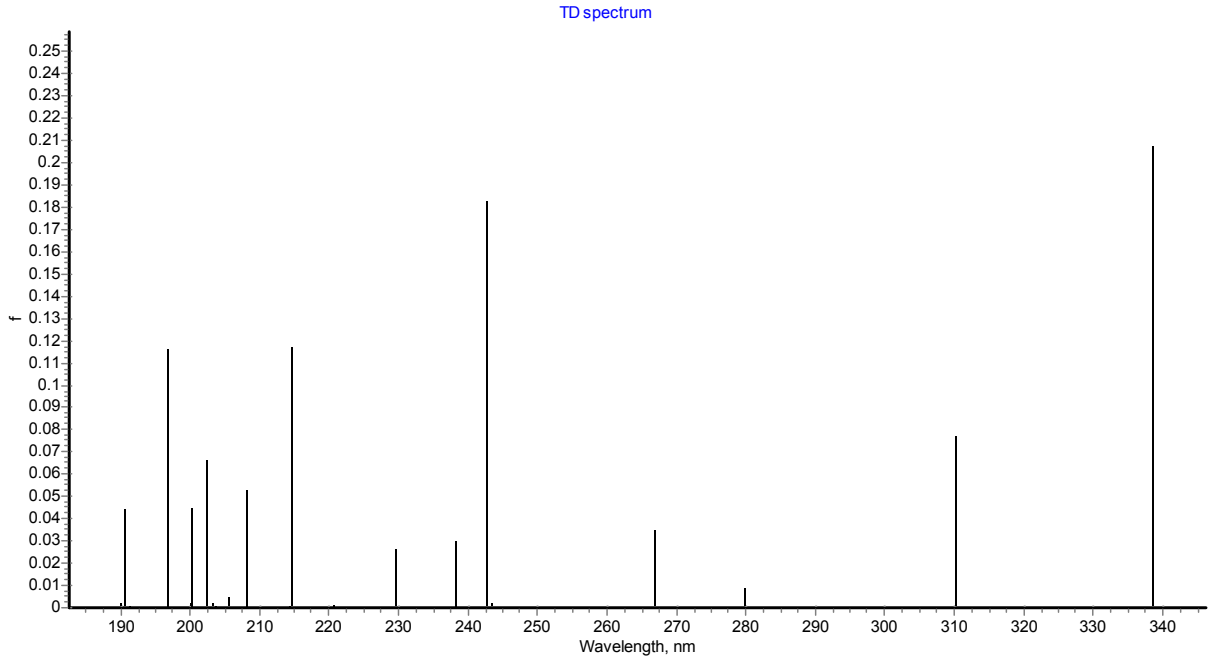
Number of vibrational modes with imaginary frequency: 1

Calculated geometry (M06/6-31+G(d,p), pcm, CH_3CN) of isoxazole 6.

7	0.744790000	-2.951270000	0.000000000
8	-0.683722000	-2.919287000	0.000000000
6	-1.103755000	-1.636080000	0.000000000
6	0.004403000	-0.839346000	0.000000000
6	1.127405000	-1.681116000	0.000000000
6	-2.389036000	-1.039603000	0.000000000
1	-3.302844000	-1.625156000	0.000000000
6	-2.427610000	0.343479000	0.000000000
1	-3.400439000	0.832255000	0.000000000
6	-1.257700000	1.180726000	0.000000000
6	0.000000000	0.540216000	0.000000000
6	2.413866000	-1.023251000	0.000000000
1	3.337869000	-1.593939000	0.000000000
6	2.437742000	0.345238000	0.000000000
1	3.405001000	0.845833000	0.000000000
6	1.253325000	1.191599000	0.000000000
6	1.223278000	2.584444000	0.000000000
1	2.149660000	3.156052000	0.000000000
6	-0.011458000	3.259724000	0.000000000
1	-0.009865000	4.346770000	0.000000000
6	-1.230791000	2.590038000	0.000000000
1	-2.161147000	3.154958000	0.000000000

E (RM06) = -629.1290972

Number of vibrational modes with imaginary frequency: 0



(TD-B3LYP/6-31+G(d,p)//M06/6-31+G(d,p), scrf=pcm, solvent=acetonitrile)

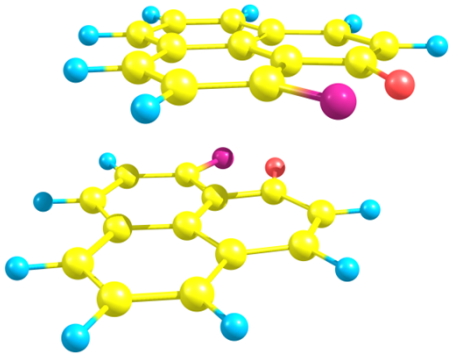
Calculated geometry (M06/6-31+G(d,p), pcm, CH_3CN) of π-dimer 1 of isoxazole 6.

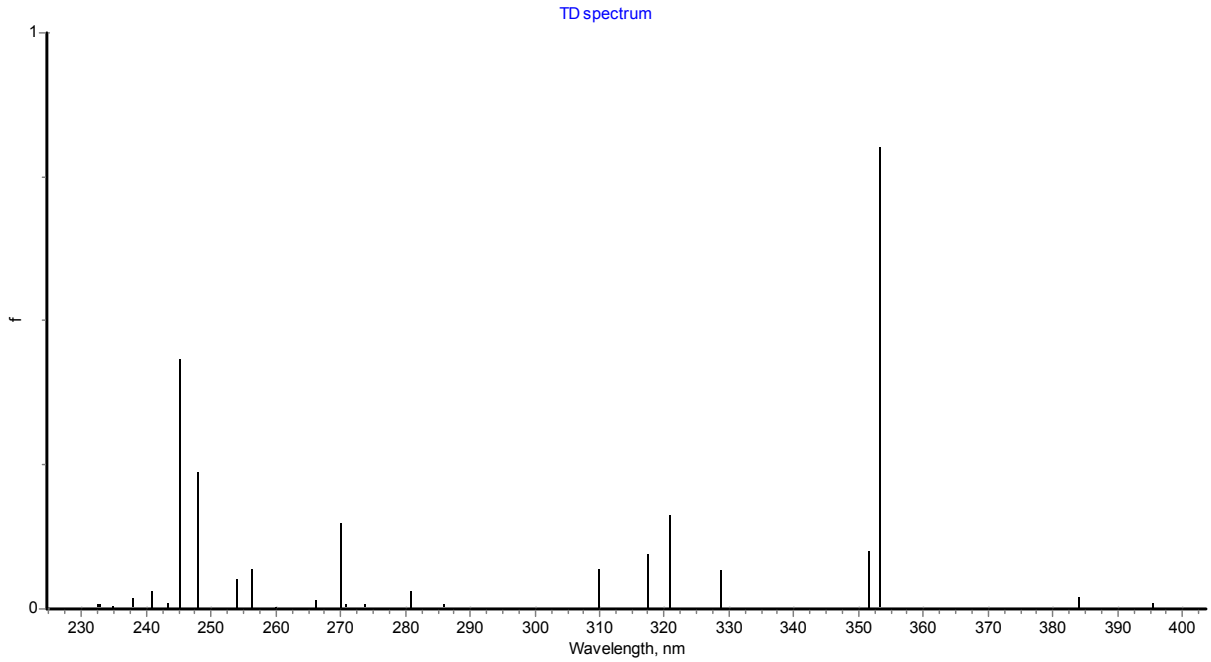
7	-2.086365000	2.990670000	0.336937000
8	-3.027130000	2.297997000	-0.488431000
6	-2.894308000	0.967769000	-0.298898000
6	-1.905036000	0.777694000	0.622045000
6	-1.427643000	2.044190000	0.993363000
6	-3.546673000	-0.157056000	-0.861093000
1	-4.340565000	-0.063907000	-1.595468000
6	-3.115092000	-1.399874000	-0.430709000
1	-3.592999000	-2.285348000	-0.846997000
6	-2.064725000	-1.596990000	0.532453000
6	-1.449544000	-0.445754000	1.069082000
6	-0.355133000	2.060700000	1.960270000
1	0.080140000	2.995241000	2.302899000
6	0.112100000	0.860115000	2.424502000
1	0.928615000	0.865439000	3.146365000
6	-0.398843000	-0.438749000	2.012846000
6	0.047161000	-1.686203000	2.444737000

1	0.858474000	-1.760960000	3.167396000
6	-0.546264000	-2.857415000	1.939549000
1	-0.176809000	-3.819451000	2.286845000
6	-1.576085000	-2.831778000	1.005083000
1	-1.996946000	-3.764527000	0.633732000
7	0.953268000	-2.946627000	-1.454326000
8	0.054100000	-2.186112000	-2.261703000
6	0.280498000	-0.868996000	-2.066293000
6	1.295632000	-0.754389000	-1.160731000
6	1.686115000	-2.054028000	-0.802194000
6	-0.306318000	0.302860000	-2.604243000
1	-1.117521000	0.270241000	-3.325330000
6	0.203823000	1.509917000	-2.158702000
1	-0.230227000	2.429912000	-2.548101000
6	1.272935000	1.626452000	-1.203263000
6	1.827792000	0.431346000	-0.698022000
6	2.758110000	-2.151097000	0.161057000
1	3.121959000	-3.115824000	0.503251000
6	3.305446000	-0.989364000	0.636472000
1	4.113904000	-1.057118000	1.363249000
6	2.879298000	0.345260000	0.240981000
6	3.401532000	1.556263000	0.692395000
1	4.215871000	1.570268000	1.414926000
6	2.871313000	2.769205000	0.216622000
1	3.290461000	3.701483000	0.587330000
6	1.829887000	2.821177000	-0.705229000
1	1.445688000	3.783641000	-1.039790000

E (RM06) = -1258.273683

Number of vibrational modes with imaginary frequency: 0





(TD-B3LYP/6-31+G(d,p)//M06/6-31+G(d,p), scrf=pcm, solvent=acetonitrile)

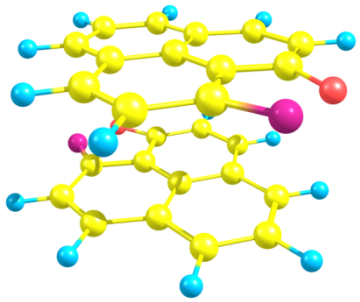
Calculated geometry (M06/6-31+G(d,p), pcm, CH_3CN) of π-dimer 2 of isoxazole 6.

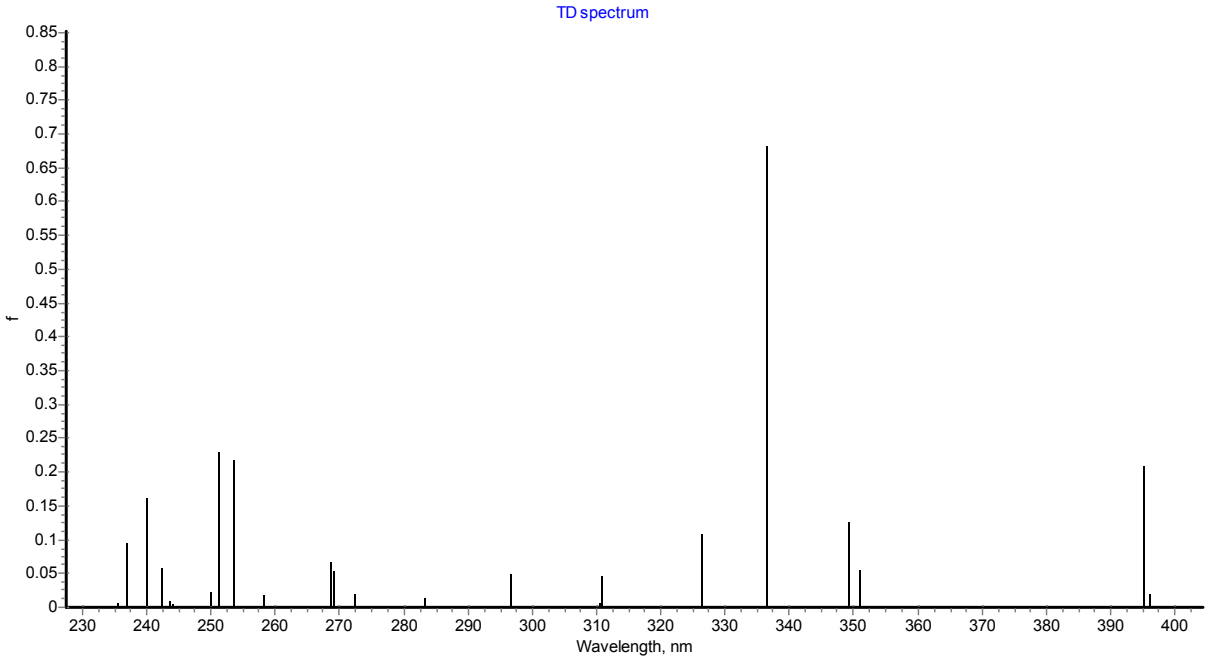
7	-3.843098000	0.764341000	-0.020572000
8	-3.822208000	-0.663975000	-0.028004000
6	-2.675473000	-1.098336000	0.538388000
6	-1.957402000	0.000635000	0.911619000
6	-2.704561000	1.132557000	0.552481000
6	-2.151680000	-2.390223000	0.790668000
1	-2.679086000	-3.297655000	0.513213000
6	-0.913077000	-2.444214000	1.405780000
1	-0.476427000	-3.422075000	1.604962000

6	-0.158411000	-1.283782000	1.797369000
6	-0.724210000	-0.019369000	1.529906000
6	-2.109645000	2.411770000	0.863716000
1	-2.612773000	3.342416000	0.616989000
6	-0.883824000	2.420420000	1.473461000
1	-0.424793000	3.381615000	1.703048000
6	-0.134529000	1.226709000	1.837087000
6	1.114388000	1.181030000	2.452624000
1	1.636938000	2.102130000	2.707834000
6	1.712629000	-0.060412000	2.734853000
1	2.692633000	-0.070631000	3.206167000
6	1.106527000	-1.271957000	2.418678000
1	1.612540000	-2.209340000	2.645806000
7	3.844229000	0.761244000	0.035263000
8	3.821725000	-0.666897000	0.014137000
6	2.674307000	-1.088533000	-0.560465000
6	1.957463000	0.018535000	-0.911518000
6	2.706022000	1.142183000	-0.530066000
6	2.149038000	-2.374540000	-0.838379000
1	2.675436000	-3.287930000	-0.579165000
6	0.910314000	-2.414834000	-1.454215000
1	0.472346000	-3.387974000	-1.672647000
6	0.156964000	-1.245964000	-1.822435000
6	0.724180000	0.012270000	-1.529918000
6	2.112553000	2.428017000	-0.815740000
1	2.616886000	3.352975000	-0.550766000
6	0.886657000	2.450216000	-1.425018000
1	0.428930000	3.416386000	-1.635589000
6	0.135802000	1.264858000	-1.812085000
6	-1.113452000	1.232759000	-2.427864000
1	-1.635185000	2.159269000	-2.664414000
6	-1.713040000	-0.002168000	-2.734671000
1	-2.693289000	-0.001867000	-3.205591000
6	-1.108060000	-1.220434000	-2.443084000
1	-1.615088000	-2.152584000	-2.688792000

E (RM06) = -1258.273683

Number of vibrational modes with imaginary frequency: 0





(TD-B3LYP/6-31+G(d,p)//M06/6-31+G(d,p), scrf=pcm, solvent=acetonitrile)

Calculated geometry (M06/6-31+G(d,p), pcm, CH_3CN) of π-dimer 3 of isoxazole 6.

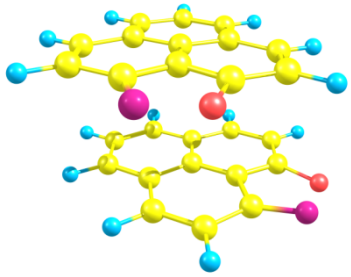
7	2.911411000	2.377725000	-0.529315000
8	1.943104000	2.998756000	0.316675000
6	1.286715000	2.050532000	1.019247000
6	1.799743000	0.838755000	0.656106000
6	2.798532000	1.075301000	-0.300817000
6	0.243808000	2.106764000	1.976589000
1	-0.204906000	3.042131000	2.296208000
6	-0.195581000	0.895027000	2.480949000

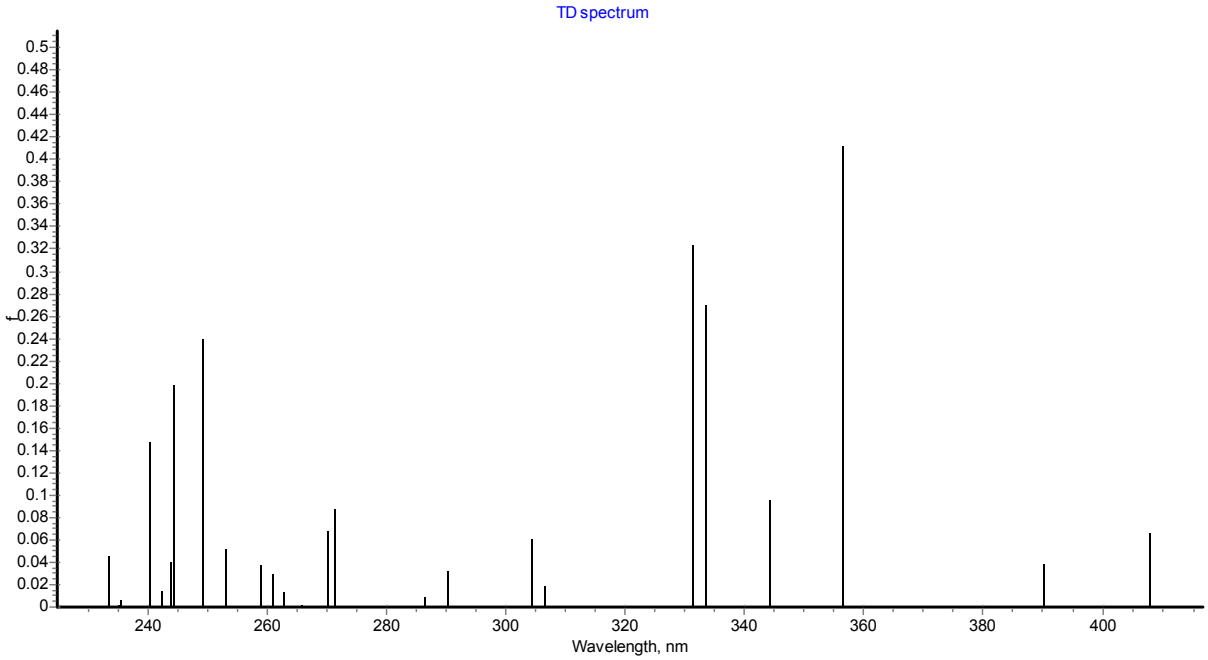
1	-1.004370000	0.902037000	3.210952000
6	0.344604000	-0.380891000	2.093715000
6	1.384783000	-0.384962000	1.140107000
6	3.463228000	-0.094271000	-0.827235000
1	4.247919000	-0.008841000	-1.573408000
6	3.071239000	-1.321411000	-0.362317000
1	3.563635000	-2.207995000	-0.760838000
6	2.028588000	-1.533653000	0.630511000
6	1.587972000	-2.757462000	1.129552000
1	2.032487000	-3.687505000	0.778394000
6	0.556033000	-2.795503000	2.085008000
1	0.225734000	-3.762806000	2.456363000
6	-0.063219000	-1.645454000	2.563754000
1	-0.864950000	-1.723168000	3.296600000
7	-2.421732000	2.730951000	-0.238573000
8	-3.232605000	1.868409000	0.561870000
6	-2.907807000	0.582635000	0.305527000
6	-1.918658000	0.586250000	-0.635105000
6	-1.641175000	1.925834000	-0.947899000
6	-3.380599000	-0.652697000	0.813007000
1	-4.164040000	-0.714072000	1.561835000
6	-2.785787000	-1.795570000	0.306705000
1	-3.121801000	-2.762003000	0.680053000
6	-1.740874000	-1.788099000	-0.681356000
6	-1.303910000	-0.533548000	-1.156604000
6	-0.599452000	2.148235000	-1.923368000
1	-0.309986000	3.152158000	-2.220841000
6	0.027146000	1.053750000	-2.456782000
1	0.821269000	1.215009000	-3.185588000
6	-0.284711000	-0.325518000	-2.111534000
6	0.324642000	-1.470905000	-2.619736000
1	1.123180000	-1.388751000	-3.355641000
6	-0.086498000	-2.740579000	-2.174995000
1	0.407584000	-3.619815000	-2.581788000
6	-1.091223000	-2.912558000	-1.228230000

1 -1.368738000 -3.914441000 -0.904241000

E (RM06) = -1258.273648

Number of vibrational modes with imaginary frequency: 0





(TD-B3LYP/6-31+G(d,p)//M06/6-31+G(d,p), scrf=pcm, solvent=acetonitrile)

Calculated geometry (M06/6-31+G(d,p), pcm, CH_3CN) of π-dimer 4 of isoxazole 6.

7 3.955214000 -0.219979000 -0.475133000

8 3.757518000 0.792683000 0.512317000

6 2.601483000 0.558764000 1.169991000

6 2.047799000 -0.571309000 0.641674000

6 2.906222000 -1.026220000 -0.370612000

6 1.934298000 1.235000000 2.221441000

1 2.329340000 2.138023000 2.676563000

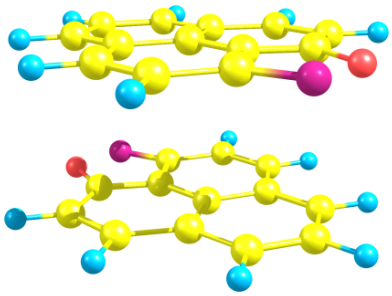
6 0.732078000 0.692480000 2.638908000

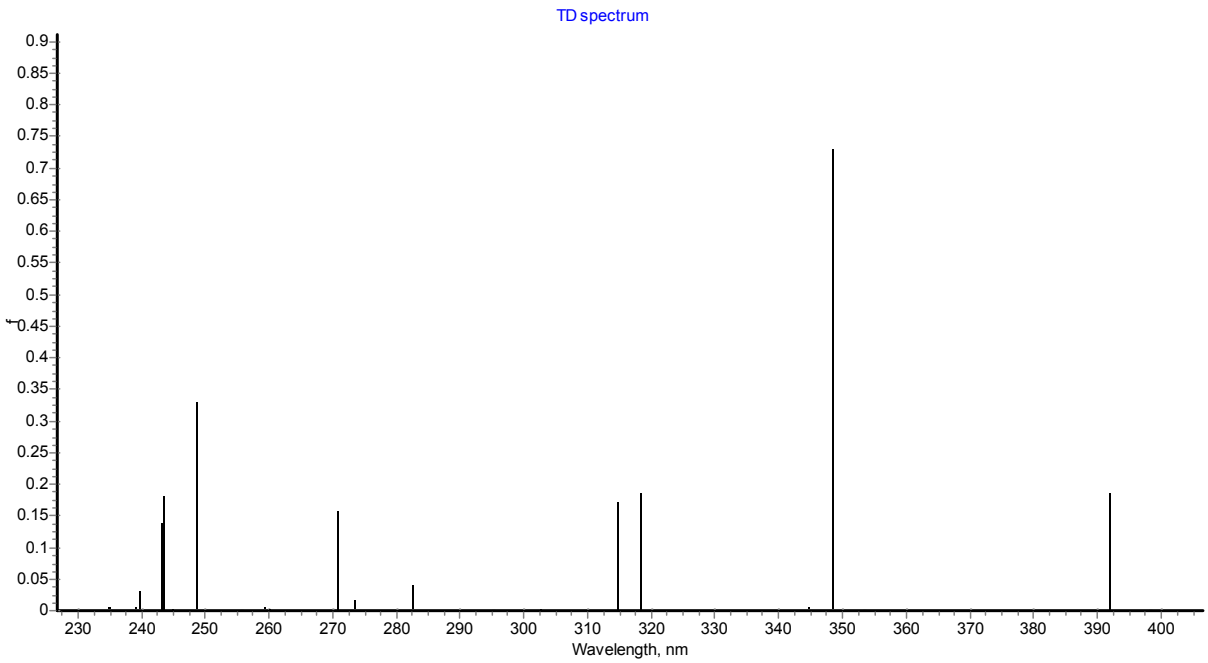
1	0.187987000	1.193919000	3.438199000
6	0.146417000	-0.494403000	2.073957000
6	0.854075000	-1.139078000	1.037215000
6	2.488892000	-2.221395000	-1.066878000
1	3.088388000	-2.646375000	-1.866765000
6	1.307527000	-2.805061000	-0.693384000
1	0.982896000	-3.701995000	-1.220046000
6	0.437096000	-2.306049000	0.360768000
6	-0.782509000	-2.847799000	0.762699000
1	-1.174662000	-3.740756000	0.277809000
6	-1.520084000	-2.231327000	1.789478000
1	-2.474887000	-2.664649000	2.077847000
6	-1.080858000	-1.082192000	2.439455000
1	-1.690300000	-0.633364000	3.222712000
7	-3.942865000	0.080541000	0.419043000
8	-3.685794000	-0.903086000	-0.583680000
6	-2.534118000	-0.604104000	-1.221266000
6	-2.039523000	0.540285000	-0.665052000
6	-2.930508000	0.935348000	0.344133000
6	-1.822237000	-1.231000000	-2.273724000
1	-2.170138000	-2.142155000	-2.750738000
6	-0.637872000	-0.629897000	-2.660824000
1	-0.059434000	-1.092400000	-3.459419000
6	-0.111738000	0.568296000	-2.062864000
6	-0.863141000	1.163927000	-1.027178000
6	-2.576067000	2.132799000	1.070300000
1	-3.205931000	2.515433000	1.868271000
6	-1.414039000	2.772865000	0.729480000
1	-1.137064000	3.671926000	1.279182000
6	-0.505336000	2.331683000	-0.318419000
6	0.697856000	2.930046000	-0.687818000
1	1.045291000	3.828058000	-0.178966000
6	1.477576000	2.364269000	-1.712797000
1	2.418252000	2.842332000	-1.975807000
6	1.097073000	1.211945000	-2.393827000

1 1.737841000 0.804049000 -3.174444000

E (RM06) = -1258.2737535

Number of vibrational modes with imaginary frequency: 0





(TD-B3LYP/6-31+G(d,p)//M06/6-31+G(d,p), scrf=pcm, solvent=acetonitrile)

Calculated geometry (M06/6-31+G(d,p), pcm, CH_3CN) of π-dimer 5 of isoxazole 6.

7 -0.273403000 -3.211796000 -0.669004000

8 -0.901051000 -2.312897000 -1.586491000

6 -0.153619000 -1.193356000 -1.698231000

6 0.934494000 -1.339311000 -0.886714000

6 0.828347000 -2.592983000 -0.265161000

6 -0.306133000 -0.002751000 -2.449625000

1 -1.153710000 0.167532000 -3.106851000

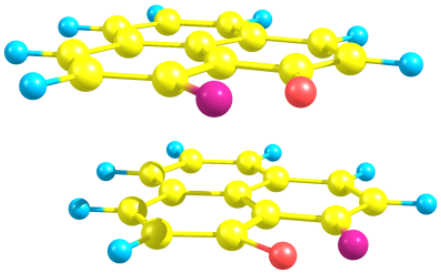
6	0.681082000	0.954760000	-2.295293000
1	0.585870000	1.888441000	-2.848679000
6	1.827902000	0.798105000	-1.440924000
6	1.936329000	-0.406445000	-0.713948000
6	1.888030000	-2.935956000	0.654484000
1	1.888598000	-3.883694000	1.185214000
6	2.896619000	-2.028790000	0.843517000
1	3.698265000	-2.282472000	1.535950000
6	2.978109000	-0.735390000	0.180951000
6	3.979324000	0.221276000	0.338417000
1	4.815820000	0.037675000	1.010596000
6	3.909280000	1.432995000	-0.372726000
1	4.700662000	2.165332000	-0.232561000
6	2.863839000	1.731924000	-1.240981000
1	2.845319000	2.687637000	-1.762564000
7	-3.998636000	-0.563110000	-0.421953000
8	-3.459627000	-1.516141000	0.495333000
6	-2.360748000	-0.999691000	1.084686000
6	-2.175450000	0.257511000	0.584362000
6	-3.202679000	0.495488000	-0.342221000
6	-1.447281000	-1.509104000	2.039439000
1	-1.540890000	-2.504762000	2.462014000
6	-0.402387000	-0.676477000	2.399556000
1	0.324430000	-1.042806000	3.123411000
6	-0.206607000	0.644721000	1.865079000
6	-1.146937000	1.112341000	0.922685000
6	-3.182418000	1.784161000	-0.995043000
1	-3.940483000	2.059187000	-1.722651000
6	-2.173983000	2.653170000	-0.674327000
1	-2.150965000	3.624382000	-1.167226000
6	-1.113077000	2.370086000	0.281146000
6	-0.052133000	3.206202000	0.623392000
1	0.045013000	4.189432000	0.165545000
6	0.906916000	2.775027000	1.557877000
1	1.732011000	3.440389000	1.801452000

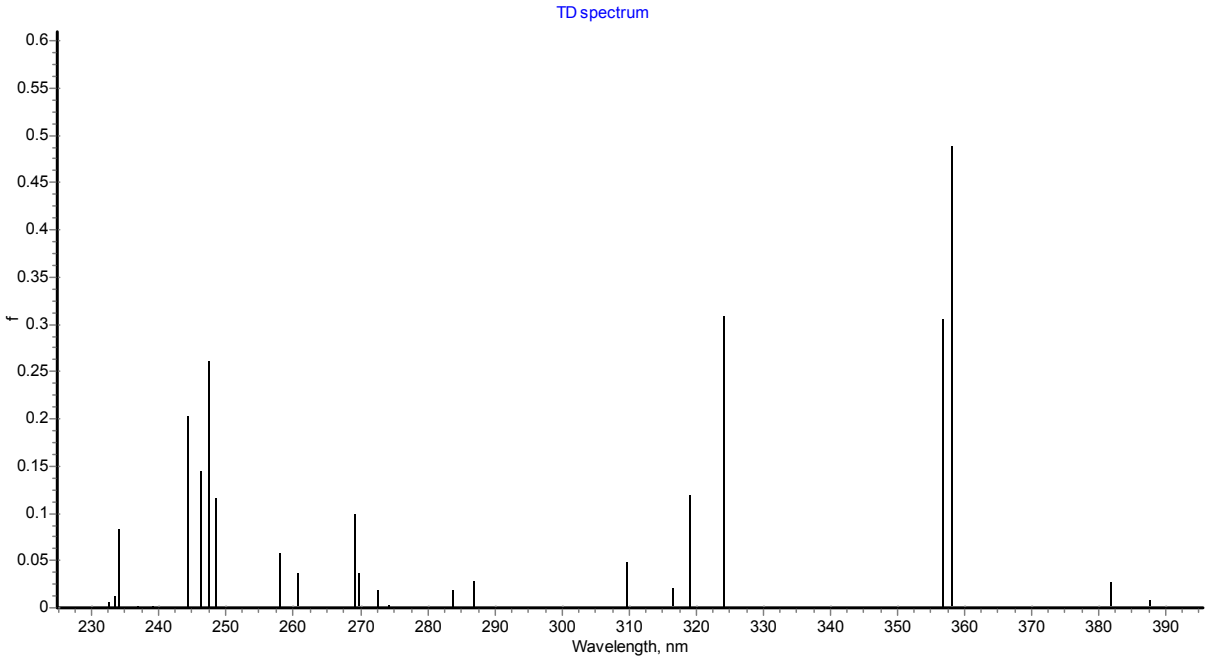
6 0.846847000 1.528589000 2.172767000

1 1.617767000 1.233754000 2.883334000

E (RM06) = -1258.2728822

Number of vibrational modes with imaginary frequency: 0





(TD-B3LYP/6-31+G(d,p)//M06/6-31+G(d,p), scrf=pcm, solvent=acetonitrile)

Calculated geometry (M06/6-31+G(d,p), pcm, CH_3CN) of π-dimer 6 of isoxazole 6.

7 -0.230783000 2.953459000 1.374283000

8 -1.212945000 3.341761000 0.412263000

6 -1.950794000 2.264852000 0.064680000

6 -1.476047000 1.195315000 0.766977000

6 -0.413751000 1.653354000 1.562273000

6 -3.030254000 2.083232000 -0.833968000

1	-3.448084000	2.898693000	-1.415909000
6	-3.535582000	0.798805000	-0.939952000
1	-4.366073000	0.625602000	-1.622478000
6	-3.027570000	-0.327905000	-0.204104000
6	-1.952597000	-0.096388000	0.680482000
6	0.242320000	0.659877000	2.380659000
1	1.078257000	0.922444000	3.023325000
6	-0.210242000	-0.630367000	2.313233000
1	0.288106000	-1.387377000	2.918595000
6	-1.315426000	-1.074653000	1.475635000
6	-1.809716000	-2.371805000	1.366498000
1	-1.363006000	-3.181366000	1.941934000
6	-2.885903000	-2.642857000	0.500761000
1	-3.253788000	-3.663837000	0.432313000
6	-3.490428000	-1.658264000	-0.273471000
1	-4.318352000	-1.915829000	-0.931666000
7	3.176173000	2.215753000	-0.097166000
8	2.174757000	2.539000000	-1.061961000
6	1.490888000	1.422642000	-1.390057000
6	2.019660000	0.388061000	-0.673152000
6	3.055573000	0.911480000	0.115745000
6	0.412101000	1.175354000	-2.275134000
1	-0.051864000	1.961752000	-2.863056000
6	-0.036237000	-0.131639000	-2.351831000
1	-0.868165000	-0.354536000	-3.018940000
6	0.525676000	-1.220233000	-1.597035000
6	1.596111000	-0.923968000	-0.726348000
6	3.748853000	-0.033264000	0.960598000
1	4.564974000	0.280229000	1.605040000
6	3.348247000	-1.342296000	0.927529000
1	3.867406000	-2.058904000	1.562683000
6	2.267019000	-1.853448000	0.097870000
6	1.818581000	-3.171629000	0.029723000
1	2.286113000	-3.944897000	0.637043000
6	0.756084000	-3.507079000	-0.828604000

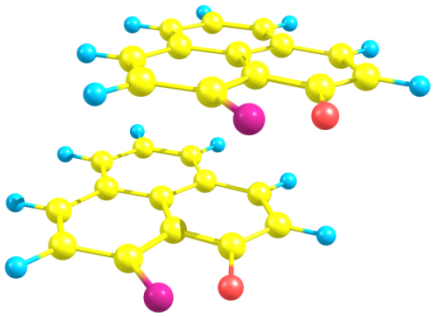
1 0.420149000 -4.540850000 -0.861974000

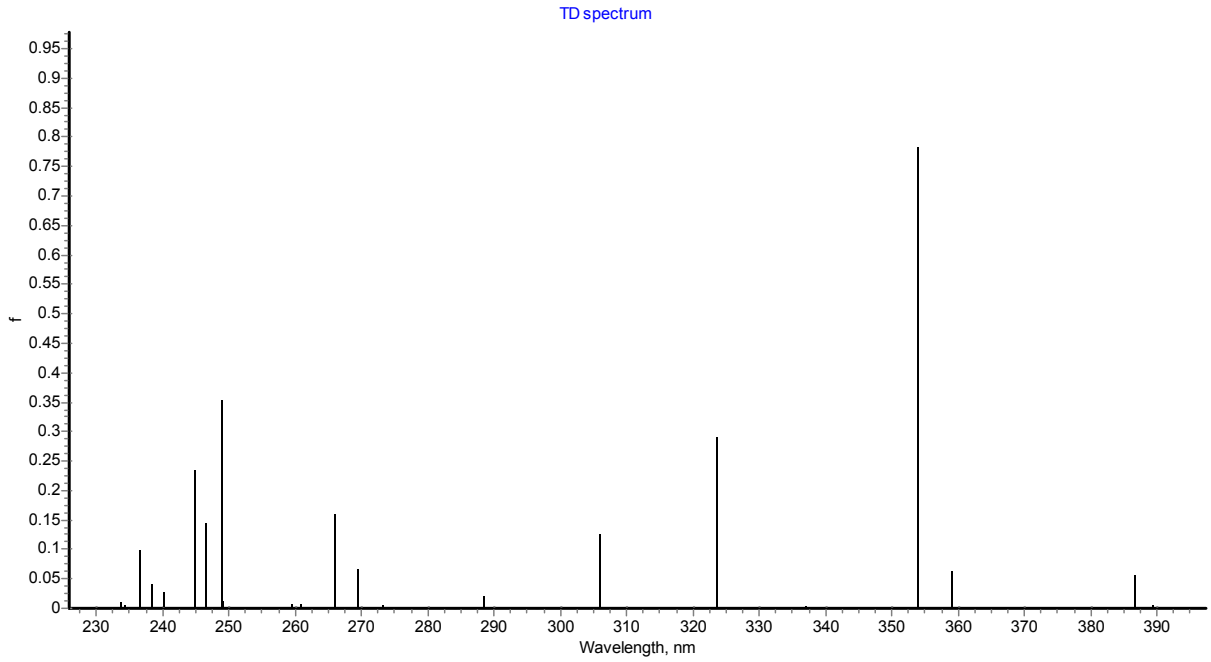
6 0.113883000 -2.567164000 -1.628630000

1 -0.710590000 -2.871767000 -2.271404000

E (RM06) = -1258.272979

Number of vibrational modes with imaginary frequency: 0





(TD-B3LYP/6-31+G(d,p)//M06/6-31+G(d,p), scrf=pcm, solvent=acetonitrile)

Calculated geometry (M06/6-31+G(d,p), pcm, CH_3CN) of π-trimer 1 of isoxazole 6.

7 -3.681640000 3.079607000 0.924152000

8 -3.607559000 3.108920000 -0.501630000

6 -3.539649000 1.845051000 -0.973088000

6 -3.575214000 1.001704000 0.099776000

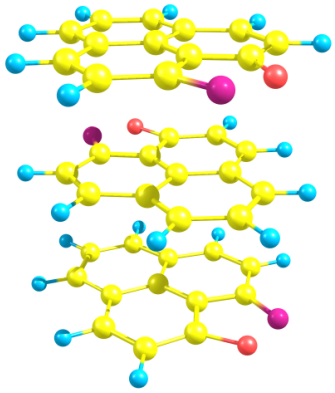
6 -3.661083000 1.794583000 1.254132000

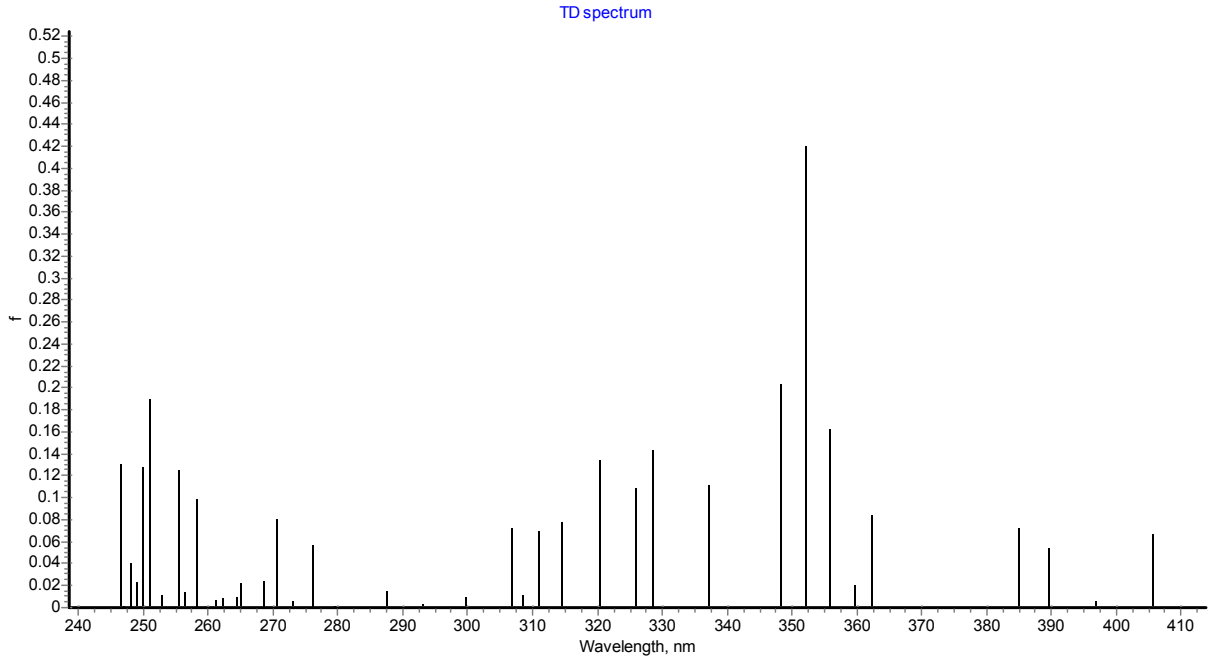
6	-3.445004000	1.305018000	-2.279219000
1	-3.408693000	1.929888000	-3.166480000
6	-3.381625000	-0.074064000	-2.374266000
1	-3.296291000	-0.521133000	-3.363825000
6	-3.411520000	-0.960093000	-1.240946000
6	-3.516208000	-0.375395000	0.039027000
6	-3.698559000	1.083613000	2.511284000
1	-3.762689000	1.613765000	3.457208000
6	-3.645824000	-0.284471000	2.479319000
1	-3.666187000	-0.826658000	3.424236000
6	-3.552773000	-1.078711000	1.263269000
6	-3.477831000	-2.467284000	1.177881000
1	-3.490536000	-3.076293000	2.080599000
6	-3.370518000	-3.087670000	-0.080125000
1	-3.301797000	-4.172111000	-0.121458000
6	-3.334334000	-2.366912000	-1.269599000
1	-3.240242000	-2.892331000	-2.218186000
7	0.141747000	-3.501177000	0.257653000
8	0.210170000	-3.356748000	-1.163232000
6	0.168557000	-2.043742000	-1.482867000
6	0.080643000	-1.339020000	-0.316802000
6	0.062789000	-2.266698000	0.736146000
6	0.195102000	-1.348409000	-2.715985000
1	0.266139000	-1.858275000	-3.671904000
6	0.128964000	0.032626000	-2.646625000
1	0.147429000	0.599475000	-3.577018000
6	0.034131000	0.772354000	-1.417051000
6	0.008203000	0.034598000	-0.214041000
6	-0.040324000	-1.714999000	2.067373000
1	-0.062730000	-2.358008000	2.943256000
6	-0.114293000	-0.354067000	2.197320000
1	-0.195090000	0.069611000	3.198579000
6	-0.097875000	0.582008000	1.083066000
6	-0.180216000	1.970918000	1.159172000
1	-0.265860000	2.464785000	2.126935000

6	-0.157061000	2.741546000	-0.017117000
1	-0.224750000	3.823635000	0.067885000
6	-0.055226000	2.171680000	-1.282380000
1	-0.044753000	2.807703000	-2.166634000
1	3.126990000	2.747077000	2.953714000
6	3.240508000	1.949951000	2.225427000
1	3.227024000	0.399766000	3.684442000
6	3.298752000	0.624932000	2.621247000
6	3.462930000	1.147157000	-0.026644000
6	3.445766000	-0.479913000	1.712123000
6	3.327457000	2.198228000	0.833568000
6	3.526933000	-0.182673000	0.335634000
6	3.508426000	-1.846522000	2.050678000
6	3.647805000	-2.802820000	1.050326000
1	3.440685000	-2.155144000	3.092720000
1	3.688002000	-3.852962000	1.329703000
6	3.731249000	-2.465997000	-0.313378000
1	3.834093000	-3.253651000	-1.058423000
6	3.666132000	-1.130442000	-0.702731000
6	3.728590000	-0.614430000	-2.063193000
1	3.825973000	-1.345378000	-2.865857000
6	3.664359000	0.712131000	-2.394560000
6	3.522600000	1.673816000	-1.326067000
1	3.711182000	1.026048000	-3.433535000
7	3.431119000	2.996969000	-1.286120000
8	3.308010000	3.329942000	0.096580000

E (RM06) = -1887.4178704

Number of vibrational modes with imaginary frequency: 0





(TD-B3LYP/6-31+G(d,p)//M06/6-31+G(d,p), scrf=pcm, solvent=acetonitrile)

All calculations, except for some of the CCSD single point energy calculations, were performed using the Gaussian09 suite of programs:

Gaussian 09, Revision **A.02**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

All stationary points optimised were characterised as minima or transition states by performing a vibrational analysis. Some CCSD single point energy calculations were performed using ORCA vers. 2.9 (citation see main paper).