

Supplementary Information

Twisted Push-Pull Ethylenes

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5-[Bis(methylthio)methylene]-2,2-dimethyl-1,3-dioxane-4,6-dione (5)

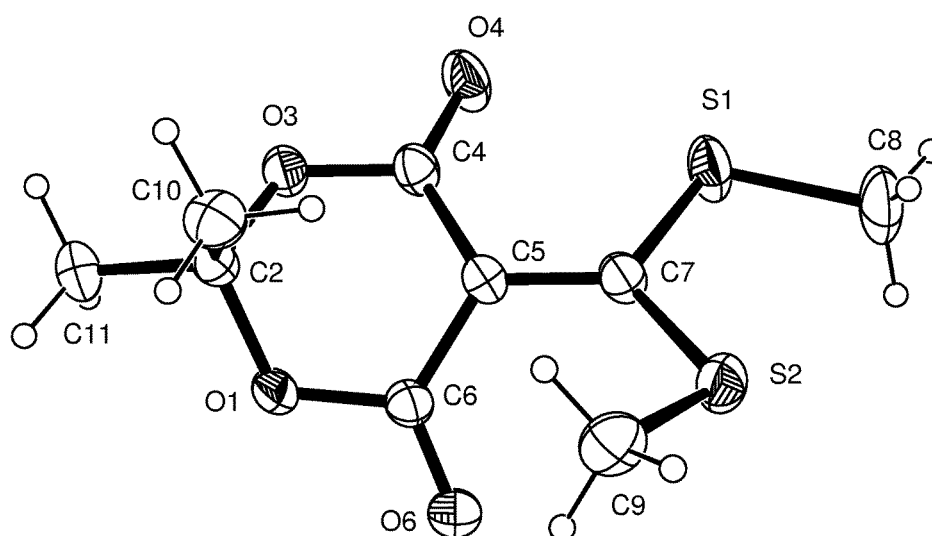


Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for r3p1479. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(2)	3198(6)	6827(4)	8784(2)	41(1)
C(4)	1899(6)	6498(4)	7294(2)	44(1)
C(5)	3149(6)	4602(4)	7434(2)	39(1)
C(6)	3300(6)	3774(4)	8410(2)	41(1)
C(7)	3725(6)	3517(4)	6687(2)	45(1)
C(8)	3364(10)	2352(6)	4940(3)	83(1)
C(9)	8072(7)	1605(5)	7464(3)	61(1)
C(10)	5861(7)	6973(5)	8501(3)	56(1)
C(11)	2032(8)	7916(5)	9587(2)	58(1)

O(1)	2944(4)	4964(3)	9072(1)	45(1)
O(3)	1715(4)	7522(3)	8018(1)	45(1)
O(4)	971(5)	7245(4)	6595(2)	67(1)
O(6)	3488(5)	2177(3)	8676(2)	60(1)
S(1)	2218(2)	4180(1)	5680(1)	65(1)
S(2)	5900(2)	1509(1)	6658(1)	57(1)

Table 2. Bond lengths [\AA] and angles [$^\circ$] for r3p1479.

C(2)-O(1)	1.428(4)
C(2)-O(3)	1.440(3)
C(2)-C(10)	1.490(5)
C(2)-C(11)	1.500(5)
C(4)-O(4)	1.210(4)
C(4)-O(3)	1.352(4)
C(4)-C(5)	1.448(4)
C(5)-C(7)	1.395(4)
C(5)-C(6)	1.467(4)
C(6)-O(6)	1.193(4)
C(6)-O(1)	1.355(4)
C(7)-S(2)	1.725(3)
C(7)-S(1)	1.733(3)
C(8)-S(1)	1.804(4)
C(9)-S(2)	1.790(4)
O(1)-C(2)-O(3)	108.5(2)
O(1)-C(2)-C(10)	111.1(3)
O(3)-C(2)-C(10)	111.1(3)
O(1)-C(2)-C(11)	107.0(3)
O(3)-C(2)-C(11)	106.0(3)
C(10)-C(2)-C(11)	112.9(3)
O(4)-C(4)-O(3)	116.9(3)
O(4)-C(4)-C(5)	126.1(3)
O(3)-C(4)-C(5)	117.0(3)
C(7)-C(5)-C(4)	120.9(3)
C(7)-C(5)-C(6)	120.9(3)
C(4)-C(5)-C(6)	117.0(3)
O(6)-C(6)-O(1)	117.7(3)

O(6)-C(6)-C(5)	125.9(3)
O(1)-C(6)-C(5)	116.0(3)
C(5)-C(7)-S(2)	125.4(2)
C(5)-C(7)-S(1)	119.7(2)
S(2)-C(7)-S(1)	114.89(18)
C(6)-O(1)-C(2)	118.9(2)
C(4)-O(3)-C(2)	118.9(2)
C(7)-S(1)-C(8)	105.09(18)
C(7)-S(2)-C(9)	106.75(17)

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for r3p1479. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

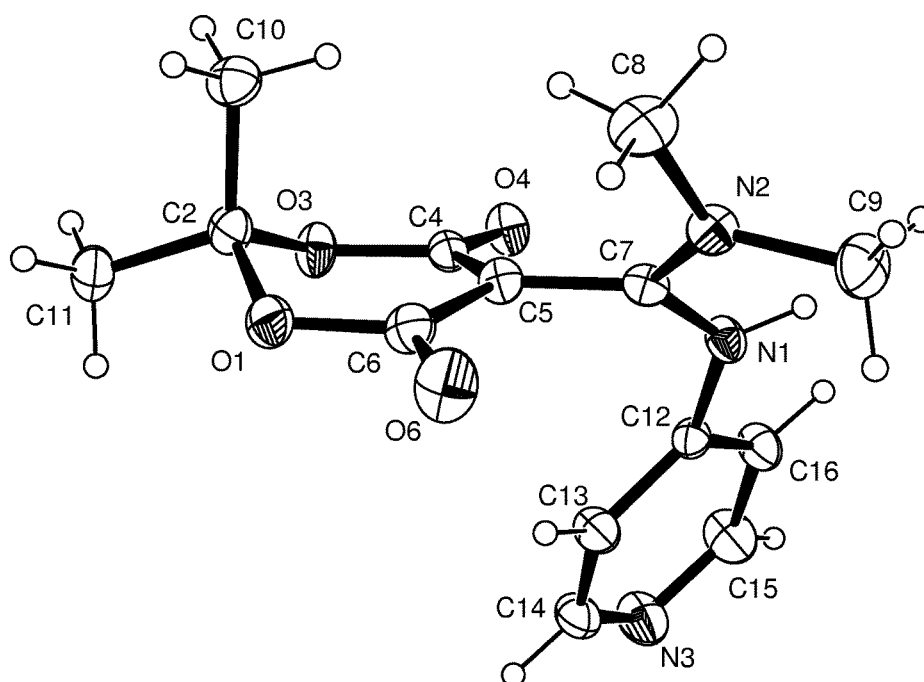
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(2)	45(2)	43(2)	34(2)	-1(1)	-7(1)	-10(1)
C(4)	43(2)	49(2)	37(2)	-9(2)	-3(1)	1(1)
C(5)	39(2)	45(2)	33(2)	-5(1)	-4(1)	-7(1)
C(6)	43(2)	43(2)	38(2)	-3(1)	-1(1)	-17(1)
C(7)	48(2)	50(2)	37(2)	-6(1)	-5(1)	-7(2)
C(8)	106(4)	86(3)	59(2)	-41(2)	-30(2)	15(3)
C(9)	50(2)	56(2)	72(3)	-5(2)	-13(2)	2(2)
C(10)	50(2)	60(2)	61(2)	-2(2)	-5(2)	-21(2)
C(11)	73(3)	63(2)	40(2)	-17(2)	-6(2)	-12(2)
O(1)	60(1)	46(1)	30(1)	-2(1)	0(1)	-20(1)
O(3)	50(1)	45(1)	38(1)	-9(1)	-7(1)	-1(1)
O(4)	84(2)	67(2)	40(1)	-12(1)	-23(1)	22(1)
O(6)	89(2)	46(2)	45(1)	0(1)	1(1)	-24(1)
S(1)	78(1)	72(1)	42(1)	-23(1)	-22(1)	16(1)
S(2)	67(1)	49(1)	53(1)	-14(1)	-12(1)	5(1)

Table 4. Torsion angles [$^\circ$] for r3p1479.

O(4)-C(4)-C(5)-C(7)	9.9(5)
O(3)-C(4)-C(5)-C(7)	-171.2(3)
O(4)-C(4)-C(5)-C(6)	-157.5(3)

O(3)-C(4)-C(5)-C(6)	21.4(4)
C(7)-C(5)-C(6)-O(6)	-13.3(5)
C(4)-C(5)-C(6)-O(6)	154.2(3)
C(7)-C(5)-C(6)-O(1)	173.6(3)
C(4)-C(5)-C(6)-O(1)	-18.9(4)
C(4)-C(5)-C(7)-S(2)	161.1(3)
C(6)-C(5)-C(7)-S(2)	-31.9(5)
C(4)-C(5)-C(7)-S(1)	-18.2(4)
C(6)-C(5)-C(7)-S(1)	148.8(3)
O(6)-C(6)-O(1)-C(2)	167.9(3)
C(5)-C(6)-O(1)-C(2)	-18.4(4)
O(3)-C(2)-O(1)-C(6)	50.5(3)
C(10)-C(2)-O(1)-C(6)	-71.9(3)
C(11)-C(2)-O(1)-C(6)	164.5(3)
O(4)-C(4)-O(3)-C(2)	-167.7(3)
C(5)-C(4)-O(3)-C(2)	13.3(4)
O(1)-C(2)-O(3)-C(4)	-47.8(3)
C(10)-C(2)-O(3)-C(4)	74.6(4)
C(11)-C(2)-O(3)-C(4)	-162.4(3)
C(5)-C(7)-S(1)-C(8)	-176.7(3)
S(2)-C(7)-S(1)-C(8)	4.0(3)
C(5)-C(7)-S(2)-C(9)	-23.8(4)
S(1)-C(7)-S(2)-C(9)	155.5(2)

5-[(4-Aminopyridyl)(dimethylamino)methylene]-2,2-dimethyl-1,3-dioxane-4,6-dione (6)



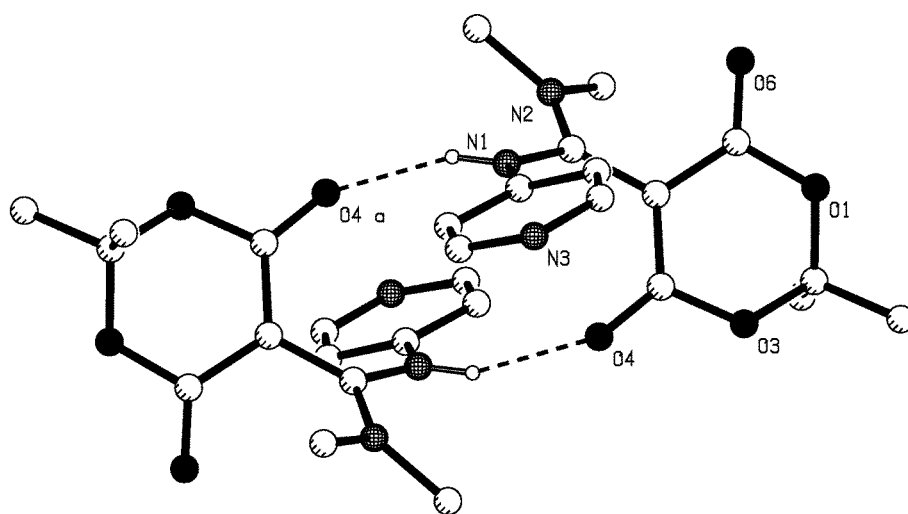


Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for r4p2484. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(2)	3417(3)	3925(2)	7674(1)	38(1)
C(4)	3618(2)	4219(2)	6407(1)	30(1)
C(5)	5169(2)	3500(2)	6470(1)	31(1)
C(6)	5555(3)	2629(2)	7083(1)	39(1)
C(7)	6281(2)	3468(2)	5885(1)	30(1)
C(8)	8635(3)	4264(3)	6627(1)	54(1)
C(9)	9069(3)	3259(3)	5428(1)	53(1)
C(10)	4372(3)	5235(2)	7921(1)	44(1)
C(11)	2044(3)	3525(3)	8164(1)	54(1)
C(12)	4326(2)	2492(2)	4976(1)	30(1)
C(13)	3611(3)	1408(2)	5367(1)	40(1)
C(14)	2248(3)	709(3)	5081(1)	47(1)
C(15)	2320(3)	1982(3)	4068(1)	56(1)
C(16)	3672(3)	2761(2)	4303(1)	41(1)
N(1)	5733(2)	3269(2)	5203(1)	34(1)
N(2)	7893(2)	3664(2)	5972(1)	37(1)

N(3)	1576(2)	965(2)	4446(1)	56(1)
O(1)	4471(2)	2696(2)	7631(1)	43(1)
O(3)	2645(2)	4189(2)	6991(1)	39(1)
O(4)	3036(2)	4853(2)	5886(1)	38(1)
O(6)	6695(2)	1781(2)	7142(1)	61(1)

Table 2. Bond lengths [Å] and angles [°] for r4p2484.

C(2)-O(1)	1.428(2)
C(2)-O(3)	1.438(2)
C(2)-C(11)	1.505(3)
C(2)-C(10)	1.509(3)
C(4)-O(4)	1.228(2)
C(4)-O(3)	1.364(2)
C(4)-C(5)	1.423(3)
C(5)-C(7)	1.435(3)
C(5)-C(6)	1.438(3)
C(6)-O(6)	1.215(2)
C(6)-O(1)	1.369(2)
C(7)-N(2)	1.322(2)
C(7)-N(1)	1.363(2)
C(8)-N(2)	1.468(3)
C(9)-N(2)	1.461(3)
C(12)-C(13)	1.381(3)
C(12)-C(16)	1.384(3)
C(12)-N(1)	1.406(2)
C(13)-C(14)	1.378(3)
C(14)-N(3)	1.324(3)
C(15)-N(3)	1.332(3)
C(15)-C(16)	1.376(3)
O(1)-C(2)-O(3)	109.60(15)
O(1)-C(2)-C(11)	106.57(18)
O(3)-C(2)-C(11)	106.19(17)
O(1)-C(2)-C(10)	111.03(17)
O(3)-C(2)-C(10)	110.39(16)
C(11)-C(2)-C(10)	112.86(17)

O(4)-C(4)-O(3)	115.74(17)
O(4)-C(4)-C(5)	127.80(17)
O(3)-C(4)-C(5)	116.46(16)
C(4)-C(5)-C(7)	120.71(16)
C(4)-C(5)-C(6)	120.41(17)
C(7)-C(5)-C(6)	118.33(17)
O(6)-C(6)-O(1)	117.17(18)
O(6)-C(6)-C(5)	126.08(19)
O(1)-C(6)-C(5)	116.61(18)
N(2)-C(7)-N(1)	115.77(17)
N(2)-C(7)-C(5)	122.25(17)
N(1)-C(7)-C(5)	121.96(16)
C(13)-C(12)-C(16)	117.59(18)
C(13)-C(12)-N(1)	123.84(17)
C(16)-C(12)-N(1)	118.45(17)
C(14)-C(13)-C(12)	118.37(19)
N(3)-C(14)-C(13)	125.3(2)
N(3)-C(15)-C(16)	124.5(2)
C(15)-C(16)-C(12)	119.0(2)
C(7)-N(1)-C(12)	126.93(16)
C(7)-N(2)-C(9)	122.12(17)
C(7)-N(2)-C(8)	122.66(18)
C(9)-N(2)-C(8)	115.19(17)
C(14)-N(3)-C(15)	115.27(19)
C(6)-O(1)-C(2)	118.05(15)
C(4)-O(3)-C(2)	118.42(15)

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for r4p2484. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(2)	43(1)	43(1)	27(1)	1(1)	-3(1)	-2(1)
C(4)	28(1)	36(1)	27(1)	-1(1)	-2(1)	-7(1)
C(5)	27(1)	37(1)	27(1)	1(1)	-6(1)	0(1)
C(6)	45(1)	39(1)	32(1)	1(1)	-5(1)	2(1)
C(7)	27(1)	30(1)	32(1)	2(1)	-6(1)	-1(1)

C(8)	37(1)	66(2)	57(1)	-12(1)	-19(1)	-4(1)
C(9)	31(1)	68(2)	59(2)	-7(1)	6(1)	1(1)
C(10)	50(1)	44(1)	39(1)	-2(1)	-8(1)	-2(1)
C(11)	65(2)	63(2)	35(1)	-5(1)	12(1)	-14(1)
C(12)	27(1)	34(1)	28(1)	-4(1)	1(1)	-2(1)
C(13)	45(1)	43(1)	32(1)	2(1)	-5(1)	-11(1)
C(14)	55(1)	47(1)	39(1)	-3(1)	3(1)	-20(1)
C(15)	59(2)	71(2)	36(1)	3(1)	-16(1)	-21(1)
C(16)	44(1)	49(1)	29(1)	5(1)	-4(1)	-12(1)
N(1)	29(1)	43(1)	29(1)	3(1)	0(1)	-8(1)
N(2)	26(1)	43(1)	41(1)	-4(1)	-5(1)	-1(1)
N(3)	53(1)	69(1)	44(1)	-2(1)	-8(1)	-26(1)
O(1)	58(1)	41(1)	30(1)	6(1)	1(1)	3(1)
O(3)	29(1)	61(1)	28(1)	-1(1)	-1(1)	-2(1)
O(4)	32(1)	51(1)	31(1)	9(1)	-5(1)	3(1)
O(6)	67(1)	64(1)	52(1)	16(1)	-1(1)	29(1)

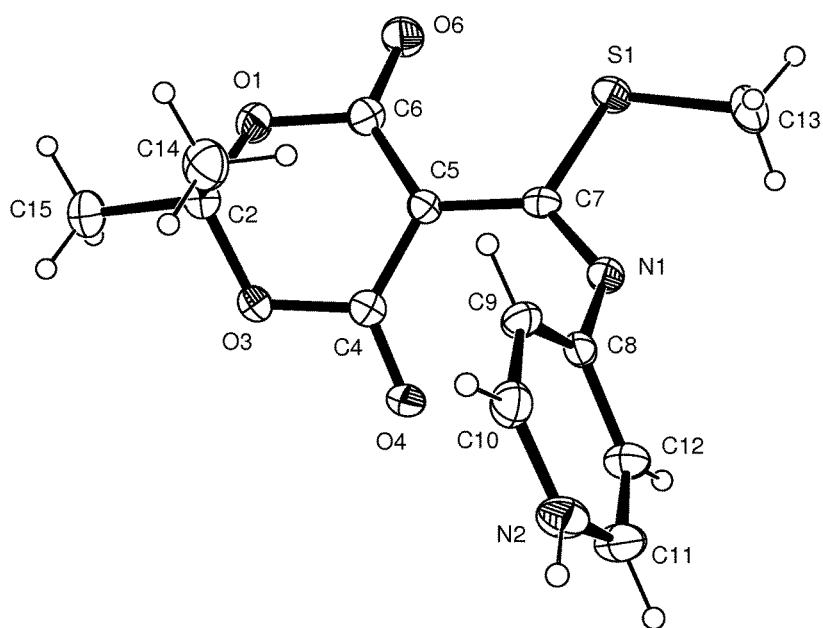
Table 4. Torsion angles [°] for r4p2484.

O(4)-C(4)-C(5)-C(7)	0.7(3)
O(3)-C(4)-C(5)-C(7)	179.89(17)
O(4)-C(4)-C(5)-C(6)	-170.70(19)
O(3)-C(4)-C(5)-C(6)	8.5(3)
C(4)-C(5)-C(6)-O(6)	166.7(2)
C(7)-C(5)-C(6)-O(6)	-4.9(3)
C(4)-C(5)-C(6)-O(1)	-8.8(3)
C(7)-C(5)-C(6)-O(1)	179.59(17)
C(4)-C(5)-C(7)-N(2)	137.7(2)
C(6)-C(5)-C(7)-N(2)	-50.7(3)
C(4)-C(5)-C(7)-N(1)	-40.6(3)
C(6)-C(5)-C(7)-N(1)	131.0(2)
C(16)-C(12)-C(13)-C(14)	-3.0(3)
N(1)-C(12)-C(13)-C(14)	-178.92(19)
C(12)-C(13)-C(14)-N(3)	1.8(4)
N(3)-C(15)-C(16)-C(12)	-0.1(4)
C(13)-C(12)-C(16)-C(15)	2.3(3)
N(1)-C(12)-C(16)-C(15)	178.4(2)

N(2)-C(7)-N(1)-C(12)	152.05(18)
C(5)-C(7)-N(1)-C(12)	-29.6(3)
C(13)-C(12)-N(1)-C(7)	-23.8(3)
C(16)-C(12)-N(1)-C(7)	160.3(2)
N(1)-C(7)-N(2)-C(9)	-18.4(3)
C(5)-C(7)-N(2)-C(9)	163.2(2)
N(1)-C(7)-N(2)-C(8)	163.41(19)
C(5)-C(7)-N(2)-C(8)	-15.0(3)
C(13)-C(14)-N(3)-C(15)	0.4(4)
C(16)-C(15)-N(3)-C(14)	-1.3(4)
O(6)-C(6)-O(1)-C(2)	162.93(18)
C(5)-C(6)-O(1)-C(2)	-21.2(3)
O(3)-C(2)-O(1)-C(6)	48.5(2)
C(11)-C(2)-O(1)-C(6)	162.99(17)
C(10)-C(2)-O(1)-C(6)	-73.7(2)
O(4)-C(4)-O(3)-C(2)	-159.04(17)
C(5)-C(4)-O(3)-C(2)	21.7(2)
O(1)-C(2)-O(3)-C(4)	-49.0(2)
C(11)-C(2)-O(3)-C(4)	-163.79(18)
C(10)-C(2)-O(3)-C(4)	73.6(2)

5-[N-(1,4-Dihydropyridin-4-ylidene)imino](methylthio)methylene]-2,2-dimethyl-1,3-dioxane-4,6-dione

(5-[(4-Pyridiniumimino)(methylthio)methyl]-2,2-dimethyl-4,6-dioxo-1,3-dioxan-5-ide) (8)



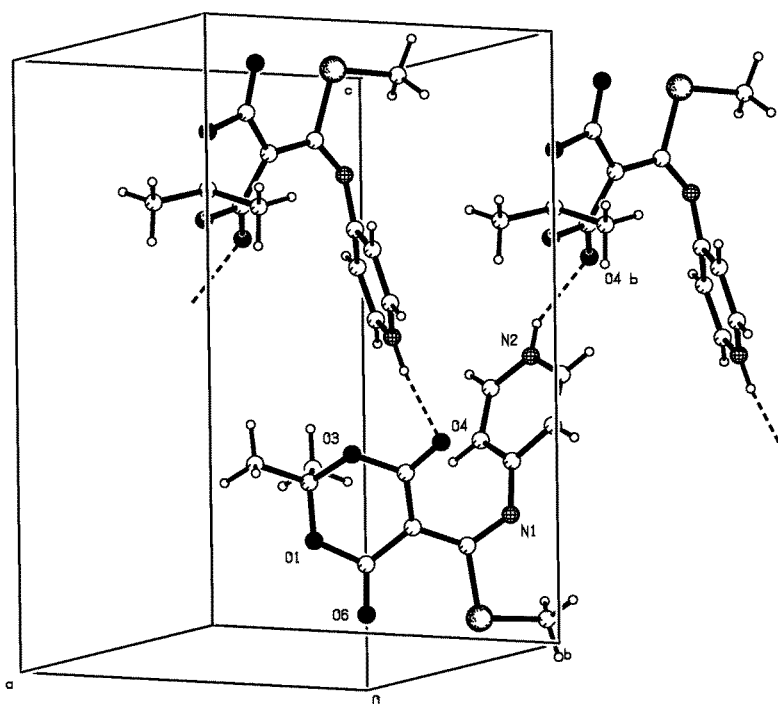


Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 053dk1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(2)	9681(3)	9464(3)	7167(2)	41(1)
C(4)	7807(3)	7812(3)	7084(2)	32(1)
C(5)	7303(2)	8390(3)	7913(2)	28(1)
C(6)	8304(3)	9032(3)	8500(2)	36(1)
C(7)	5855(3)	8179(2)	8188(2)	28(1)
C(8)	4632(3)	8001(2)	6782(2)	31(1)
C(9)	4833(2)	9251(3)	6351(2)	35(1)
C(10)	4432(3)	9419(3)	5475(2)	41(1)
C(11)	3613(3)	7190(3)	5399(2)	47(1)
C(12)	4007(3)	6975(3)	6259(2)	39(1)
C(13)	3514(2)	8308(3)	9310(2)	57(1)
C(14)	8891(3)	10686(3)	6822(2)	54(1)
C(15)	11239(3)	9455(3)	6915(2)	61(1)
N(1)	4803(2)	7795(2)	7679(1)	35(1)
N(2)	3824(2)	8407(2)	5012(1)	44(1)
O(1)	9611(2)	9371(2)	8126(1)	43(1)

O(3)	9111(2)	8241(2)	6786(1)	40(1)
O(4)	7273(2)	6908(2)	6633(1)	39(1)
O(6)	8167(2)	9292(2)	9297(1)	50(1)
S(1)	5419(1)	8378(1)	9345(1)	40(1)

Table 2. Bond lengths [\AA] and angles [$^\circ$] for 053dk1.

C(2)-O(1)	1.424(3)
C(2)-O(3)	1.440(3)
C(2)-C(14)	1.509(4)
C(2)-C(15)	1.512(3)
C(4)-O(4)	1.224(3)
C(4)-O(3)	1.370(3)
C(4)-C(5)	1.436(3)
C(5)-C(6)	1.430(3)
C(5)-C(7)	1.436(3)
C(6)-O(6)	1.215(3)
C(6)-O(1)	1.389(3)
C(7)-N(1)	1.300(3)
C(7)-S(1)	1.773(2)
C(8)-N(1)	1.353(3)
C(8)-C(12)	1.407(3)
C(8)-C(9)	1.407(3)
C(9)-C(10)	1.360(3)
C(10)-N(2)	1.343(3)
C(11)-C(12)	1.344(3)
C(11)-N(2)	1.349(3)
C(13)-S(1)	1.792(2)
O(1)-C(2)-O(3)	108.6(2)
O(1)-C(2)-C(14)	111.5(2)
O(3)-C(2)-C(14)	111.1(2)
O(1)-C(2)-C(15)	106.9(2)
O(3)-C(2)-C(15)	105.0(2)
C(14)-C(2)-C(15)	113.5(3)
O(4)-C(4)-O(3)	114.8(2)
O(4)-C(4)-C(5)	128.5(2)

O(3)-C(4)-C(5)	116.5(2)
C(6)-C(5)-C(4)	118.7(2)
C(6)-C(5)-C(7)	121.1(2)
C(4)-C(5)-C(7)	119.8(2)
O(6)-C(6)-O(1)	115.4(3)
O(6)-C(6)-C(5)	127.9(3)
O(1)-C(6)-C(5)	116.6(2)
N(1)-C(7)-C(5)	126.9(2)
N(1)-C(7)-S(1)	114.59(18)
C(5)-C(7)-S(1)	118.47(19)
N(1)-C(8)-C(12)	118.7(2)
N(1)-C(8)-C(9)	124.2(2)
C(12)-C(8)-C(9)	116.3(2)
C(10)-C(9)-C(8)	120.2(2)
N(2)-C(10)-C(9)	120.9(3)
C(12)-C(11)-N(2)	120.2(3)
C(11)-C(12)-C(8)	121.5(3)
C(7)-N(1)-C(8)	127.9(2)
C(10)-N(2)-C(11)	120.9(2)
C(6)-O(1)-C(2)	117.0(2)
C(4)-O(3)-C(2)	117.9(2)
C(7)-S(1)-C(13)	101.50(13)

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 053dk1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(2)	36(2)	45(2)	41(2)	-6(2)	5(2)	-6(2)
C(4)	31(2)	32(2)	32(2)	2(1)	-3(1)	5(2)
C(5)	27(1)	31(1)	27(2)	0(1)	-1(1)	3(2)
C(6)	31(2)	36(2)	40(2)	1(2)	-4(2)	5(1)
C(7)	40(2)	20(1)	25(1)	1(1)	-2(1)	2(1)
C(8)	23(1)	41(2)	27(2)	-4(1)	1(1)	1(2)
C(9)	35(2)	41(2)	28(2)	-3(2)	-5(1)	-7(2)
C(10)	39(2)	41(2)	44(2)	2(2)	3(2)	-4(2)
C(11)	60(2)	42(2)	39(2)	-8(2)	-5(2)	-7(2)

C(12)	51(2)	36(2)	31(2)	-2(2)	-3(2)	-2(2)
C(13)	45(2)	78(2)	49(2)	-5(2)	17(2)	-5(2)
C(14)	61(2)	46(2)	55(2)	11(2)	10(2)	-4(2)
C(15)	39(2)	71(2)	72(3)	-14(2)	16(2)	-10(2)
N(1)	35(1)	43(1)	27(1)	-2(1)	1(1)	-4(1)
N(2)	53(2)	53(1)	26(1)	0(2)	-7(1)	4(2)
O(1)	31(1)	56(1)	43(1)	-6(1)	-2(1)	-7(1)
O(3)	33(1)	44(1)	43(1)	-11(1)	10(1)	-2(1)
O(4)	39(1)	41(1)	37(1)	-12(1)	3(1)	0(1)
O(6)	48(1)	75(1)	28(1)	-8(1)	-4(1)	-8(1)
S(1)	45(1)	50(1)	25(1)	-2(1)	3(1)	-4(1)

Table 4. Torsion angles [°] for 053dk1.

O(4)-C(4)-C(5)-C(6)	156.0(3)
O(3)-C(4)-C(5)-C(6)	-18.2(3)
O(4)-C(4)-C(5)-C(7)	-16.7(4)
O(3)-C(4)-C(5)-C(7)	169.1(2)
C(4)-C(5)-C(6)-O(6)	-161.4(3)
C(7)-C(5)-C(6)-O(6)	11.2(4)
C(4)-C(5)-C(6)-O(1)	16.8(3)
C(7)-C(5)-C(6)-O(1)	-170.6(2)
C(6)-C(5)-C(7)-N(1)	169.2(2)
C(4)-C(5)-C(7)-N(1)	-18.3(4)
C(6)-C(5)-C(7)-S(1)	-13.8(3)
C(4)-C(5)-C(7)-S(1)	158.68(18)
N(1)-C(8)-C(9)-C(10)	-170.0(2)
C(12)-C(8)-C(9)-C(10)	0.0(4)
C(8)-C(9)-C(10)-N(2)	0.9(4)
N(2)-C(11)-C(12)-C(8)	0.7(4)
N(1)-C(8)-C(12)-C(11)	169.8(3)
C(9)-C(8)-C(12)-C(11)	-0.7(4)
C(5)-C(7)-N(1)-C(8)	-28.3(4)
S(1)-C(7)-N(1)-C(8)	154.7(2)
C(12)-C(8)-N(1)-C(7)	143.1(2)
C(9)-C(8)-N(1)-C(7)	-47.2(4)
C(9)-C(10)-N(2)-C(11)	-0.9(4)
C(12)-C(11)-N(2)-C(10)	0.1(4)

O(6)-C(6)-O(1)-C(2)	-161.8(2)
C(5)-C(6)-O(1)-C(2)	19.8(3)
O(3)-C(2)-O(1)-C(6)	-51.8(3)
C(14)-C(2)-O(1)-C(6)	70.8(3)
C(15)-C(2)-O(1)-C(6)	-164.6(2)
O(4)-C(4)-O(3)-C(2)	168.2(2)
C(5)-C(4)-O(3)-C(2)	-16.8(3)
O(1)-C(2)-O(3)-C(4)	50.6(3)
C(14)-C(2)-O(3)-C(4)	-72.3(3)
C(15)-C(2)-O(3)-C(4)	164.7(2)
N(1)-C(7)-S(1)-C(13)	-12.3(2)
C(5)-C(7)-S(1)-C(13)	170.4(2)

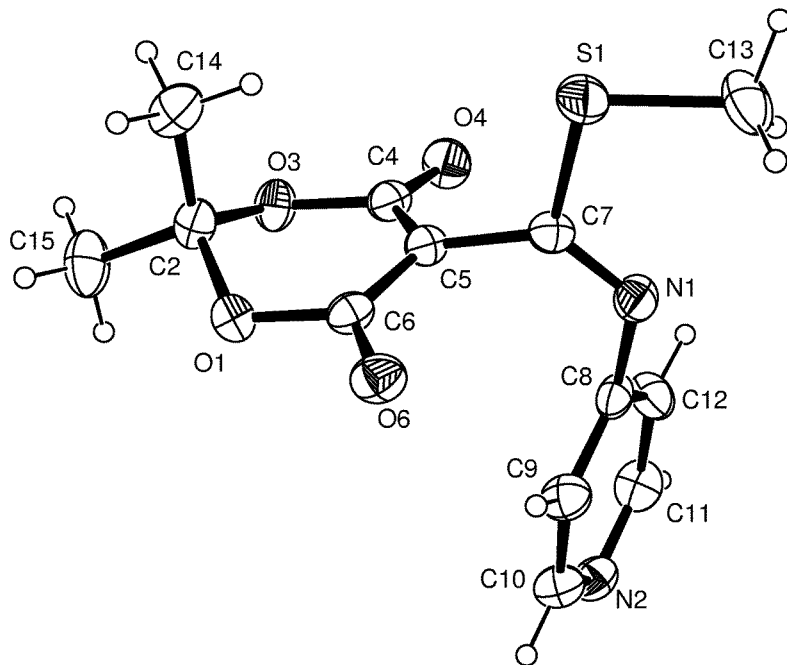
Table 5. Hydrogen bonds for 053dk1 [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
N(2)-H(2)...O(4)#1	0.86	2.07	2.856(3)	151.0

Symmetry transformations used to generate equivalent atoms:

#1 $x-1/2, -y+3/2, -z+1$

4-Aminopyridinium salt of 5-[(4-pyridylimino)(methylthio)methyl]-2,2-dimethyl-4,6-dioxo-1,3-dioxan-5-ide (9)



The 4-aminopyridinium cation is numbered N4(H)-C18-C17-C16(N3(H₂))-C20-C19.

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for r4p1480. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x
C(2)	276(3)
C(4)	1411(3)
C(5)	1498(2)
C(6)	1221(2)
C(7)	1967(3)
C(8)	3498(3)
C(9)	3609(3)
C(10)	4329(3)
C(11)	4818(3)
C(12)	4135(3)

C(13)	1935(3)
C(14)	-598(3)
C(15)	57(3)
C(16)	7586(3)
C(17)	7085(3)
C(18)	6516(3)
C(19)	6887(3)
C(20)	7477(3)
N(1)	2838(2)
N(2)	4935(2)
N(3)	8129(2)
N(4)	6406(2)
O(1)	754(2)
O(3)	884(2)
O(4)	1769(2)
O(6)	1399(2)
S(1)	1174(1)

Table 2. Bond lengths [\AA] and angles [$^\circ$] for r4p1480.

C(2)-O(1)	1.423(4)
C(2)-O(3)	1.431(4)
C(2)-C(15)	1.513(5)
C(2)-C(14)	1.515(5)
C(4)-O(4)	1.230(4)
C(4)-O(3)	1.390(4)
C(4)-C(5)	1.400(5)
C(5)-C(6)	1.394(5)
C(5)-C(7)	1.473(5)
C(6)-O(6)	1.235(4)
C(6)-O(1)	1.379(4)
C(7)-N(1)	1.271(4)
C(7)-S(1)	1.753(4)
C(8)-C(9)	1.371(5)
C(8)-C(12)	1.373(5)
C(8)-N(1)	1.400(5)
C(9)-C(10)	1.377(5)

C(10)-N(2)	1.329(5)
C(11)-N(2)	1.316(5)
C(11)-C(12)	1.367(5)
C(13)-S(1)	1.790(4)
C(16)-N(3)	1.325(5)
C(16)-C(17)	1.405(5)
C(16)-C(20)	1.409(5)
C(17)-C(18)	1.348(5)
C(18)-N(4)	1.331(5)
C(19)-N(4)	1.338(5)
C(19)-C(20)	1.340(5)
O(1)-C(2)-O(3)	110.4(3)
O(1)-C(2)-C(15)	106.8(4)
O(3)-C(2)-C(15)	106.0(3)
O(1)-C(2)-C(14)	110.5(3)
O(3)-C(2)-C(14)	110.4(3)
C(15)-C(2)-C(14)	112.6(4)
O(4)-C(4)-O(3)	115.8(4)
O(4)-C(4)-C(5)	127.8(4)
O(3)-C(4)-C(5)	116.4(3)
C(6)-C(5)-C(4)	121.9(3)
C(6)-C(5)-C(7)	119.3(3)
C(4)-C(5)-C(7)	118.6(3)
O(6)-C(6)-O(1)	116.0(4)
O(6)-C(6)-C(5)	126.9(4)
O(1)-C(6)-C(5)	116.9(3)
N(1)-C(7)-C(5)	128.4(3)
N(1)-C(7)-S(1)	119.2(3)
C(5)-C(7)-S(1)	112.4(3)
C(9)-C(8)-C(12)	116.6(4)
C(9)-C(8)-N(1)	124.0(4)
C(12)-C(8)-N(1)	119.1(4)
C(8)-C(9)-C(10)	119.6(4)
N(2)-C(10)-C(9)	124.0(4)
N(2)-C(11)-C(12)	124.6(4)
C(11)-C(12)-C(8)	119.7(4)
N(3)-C(16)-C(17)	121.4(4)

N(3)-C(16)-C(20)	121.8(4)
C(17)-C(16)-C(20)	116.8(4)
C(18)-C(17)-C(16)	119.6(4)
N(4)-C(18)-C(17)	122.0(4)
N(4)-C(19)-C(20)	121.9(4)
C(19)-C(20)-C(16)	119.8(4)
C(7)-N(1)-C(8)	121.2(3)
C(11)-N(2)-C(10)	115.4(3)
C(18)-N(4)-C(19)	119.9(4)
C(6)-O(1)-C(2)	116.6(3)
C(4)-O(3)-C(2)	117.6(3)
C(7)-S(1)-C(13)	102.29(18)

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for r4p1480. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U11
C(2)	46(2)
C(4)	41(2)
C(5)	39(2)
C(6)	36(2)
C(7)	44(2)
C(8)	33(2)
C(9)	43(2)
C(10)	47(2)
C(11)	51(3)
C(12)	60(3)
C(13)	73(3)
C(14)	47(3)
C(15)	82(3)
C(16)	46(2)
C(17)	64(3)
C(18)	72(3)
C(19)	78(3)
C(20)	70(3)
N(1)	45(2)

N(2)	40(2)
N(3)	83(3)
N(4)	58(2)
O(1)	52(2)
O(3)	54(2)
O(4)	67(2)
O(6)	57(2)
S(1)	50(1)

Table 4. Torsion angles [°] for r4p1480.

O(4)-C(4)-C(5)-C(6)	-166.4(4)
O(3)-C(4)-C(5)-C(6)	11.2(5)
O(4)-C(4)-C(5)-C(7)	8.6(6)
O(3)-C(4)-C(5)-C(7)	-173.9(3)
C(4)-C(5)-C(6)-O(6)	167.7(4)
C(7)-C(5)-C(6)-O(6)	-7.3(6)
C(4)-C(5)-C(6)-O(1)	-7.4(5)
C(7)-C(5)-C(6)-O(1)	177.6(3)
C(6)-C(5)-C(7)-N(1)	88.7(5)
C(4)-C(5)-C(7)-N(1)	-86.4(5)
C(6)-C(5)-C(7)-S(1)	-93.0(4)
C(4)-C(5)-C(7)-S(1)	91.9(4)
C(12)-C(8)-C(9)-C(10)	-0.5(6)
N(1)-C(8)-C(9)-C(10)	-174.7(4)
C(8)-C(9)-C(10)-N(2)	-0.9(6)
N(2)-C(11)-C(12)-C(8)	-1.5(6)
C(9)-C(8)-C(12)-C(11)	1.6(6)
N(1)-C(8)-C(12)-C(11)	176.1(4)
N(3)-C(16)-C(17)-C(18)	177.8(4)
C(20)-C(16)-C(17)-C(18)	-1.7(6)
C(16)-C(17)-C(18)-N(4)	-0.5(6)
N(4)-C(19)-C(20)-C(16)	-1.5(6)
N(3)-C(16)-C(20)-C(19)	-176.8(4)
C(17)-C(16)-C(20)-C(19)	2.6(6)
C(5)-C(7)-N(1)-C(8)	-1.2(6)
S(1)-C(7)-N(1)-C(8)	-179.4(3)
C(9)-C(8)-N(1)-C(7)	-72.4(5)

C(12)-C(8)-N(1)-C(7)	113.6(4)
C(12)-C(11)-N(2)-C(10)	0.1(6)
C(9)-C(10)-N(2)-C(11)	1.1(6)
C(17)-C(18)-N(4)-C(19)	1.8(6)
C(20)-C(19)-N(4)-C(18)	-0.8(6)
O(6)-C(6)-O(1)-C(2)	160.0(3)
C(5)-C(6)-O(1)-C(2)	-24.3(4)
O(3)-C(2)-O(1)-C(6)	49.9(4)
C(15)-C(2)-O(1)-C(6)	164.7(3)
C(14)-C(2)-O(1)-C(6)	-72.6(4)
O(4)-C(4)-O(3)-C(2)	-165.3(3)
C(5)-C(4)-O(3)-C(2)	16.8(5)
O(1)-C(2)-O(3)-C(4)	-46.1(4)
C(15)-C(2)-O(3)-C(4)	-161.4(3)
C(14)-C(2)-O(3)-C(4)	76.5(4)
N(1)-C(7)-S(1)-C(13)	1.2(4)
C(5)-C(7)-S(1)-C(13)	-177.3(3)

Table 5. Hydrogen bonds for r4p1480 [\AA and $^\circ$].

D-H...A	d(D-H)
N(3)-H(3A)...O(4)#1	0.86
N(3)-H(3B)...O(6)#2	0.86
N(4)-H(4)...N(2)	0.86

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1, y-1/2, -z+1/2$ #2 $-x+1, -y+1, -z+1$

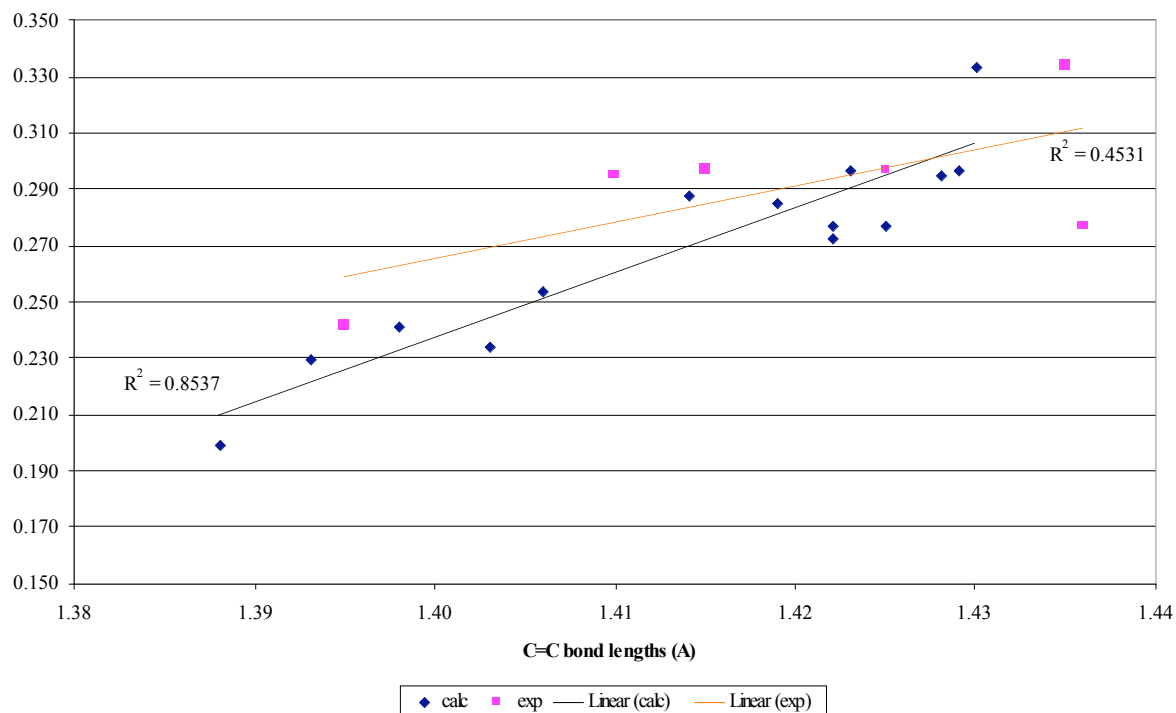


Figure S1. Graph of π^*/π orbital occupation quotients of the central C5=C7 bond (ordinate) vs. bond lengths using the method of Kleinpeter et al.,¹ calculated at the B3LYP/6-31G(d)(SCRF) level.

The correlation between bond lengths and π^*/π quotients (Figure S1) is much better, although not perfect ($R^2 = 0.8505$) when comparing orbital occupation with computed bond lengths, regardless of their origin (gas phase or SCRF). When using the SCRF π^*/π quotients together with the experimental data, the correlation is poor ($R^2 = 0.4764$).

In the case of compounds **11** (C=C = 1.410 Å) and **12** (C=C = 1.415 Å), the intramolecular hydrogen bonds lengthen the C5=C7 bonds,² but theory predicts even longer bonds (1.428 and 1.423 Å). Shorter C5=C7 bonds would lead to an even poorer correlation. In the case of compound **10** (C=C = 1.425 Å), theory predicts the bond length correctly (1.429 Å). In the case of compound **9**, the C5C7 bond (1.437 Å) is longer than predicted by theory.

¹ E. Kleinpeter, A. Schulenburg, *Tetrahedron Lett.*, **2005**, 46, 5995. E. Kleinpeter, S. Klod, W.-D. Rudorf, *J. Org. Chem.* **2004**, 69, 4317.

² I. Alkorta, C. Wentrup and J. Elguero, *J. Mol. Struct. (THEOCHEM)*, **2002**, 585, 27.

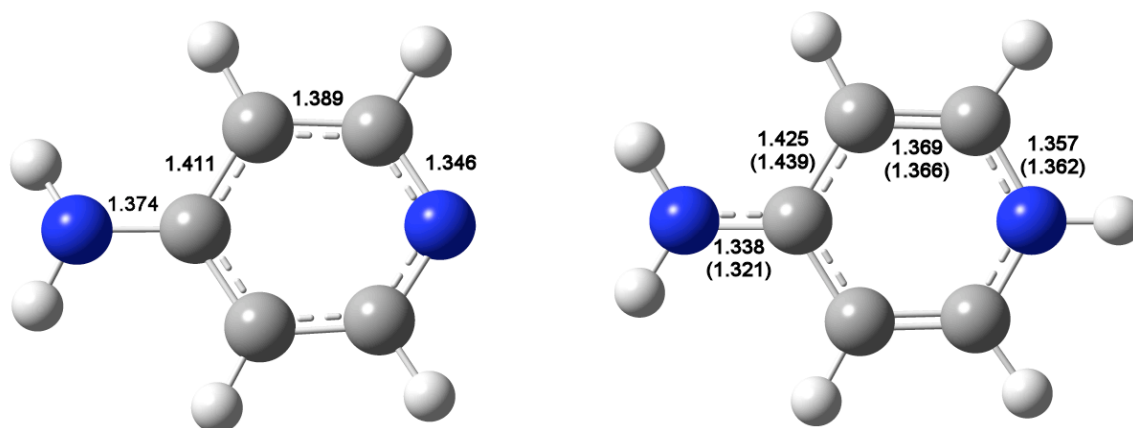


Figure S2. Selected PCM-B3LYP/6-31G(d)-computed bond lengths (Å) of 4-aminopyridine (left) and 4-aminopyridinium cation (right). Values in parenthesis are for the 4-aminopyridinium moiety in compound **8**.

Table S1. Selected PCM-B3LYP/6-31G(d)-computed NPA charges of 4-aminopyridine, 4-aminopyridinium cation, and compound **8** (atom numbering in the structure of **8** is used)

	N1	C8	C9	C10	N2	H(N2)	H(C9)	H(C10)
4-aminopyridine	-0.835	0.199	-0.338	0.013	-0.546	-	0.254	0.231
4-amino-pyridinium cation	-0.767	0.247	-0.314	0.055	-0.522	0.507	0.285	0.284
8	-0.534	0.253	-0.312	0.033	-0.538	0.496	0.271	0.273

Computational data

The following entries consist of the label, according to the main manuscript, the total energy in Hartrees at a given level of theory and the cartesian coordinates of the optimised structure. A label of **x-SCRF** refers to a structure optimised in a solvent field.

3

B3LYP/6-31G(d) energy (a.u.): -847.1925262

C 1.9660963231 1.3264795652 -0.5404764643
C 1.2865031765 0.0802042336 -0.2667628631
C 3.4833269247 1.3971012609 -0.510994526
C 1.0165418684 -2.3080669674 0.6412354732
C 1.9051603972 -1.1253209988 0.2210067095
O 1.311717628 2.3656231444 -0.7810479439
O 3.1304246475 -1.2896129453 0.3210061048
C -0.1748622346 0.2445470008 -0.3691801685
N -0.9164756897 0.4702968009 0.7388918635
C -2.3671879685 0.6598886036 0.6246218936
N -0.7909166578 0.208961032 -1.5684917753
C -2.6515278476 1.5377955093 -0.5867334308
C -0.2887967027 0.8128001785 2.0462114758
C -0.1758603539 -0.2762730031 -2.8475986497
C -0.365499819 2.323027405 2.3115833002
C -0.8773669624 -0.0323281896 3.1810341148
C 0.7448429121 0.752432831 -3.517103651
C -2.116385958 0.8164808074 -1.8102590501
C 0.4541705549 -1.6708321668 -2.7719342881
H 3.9315597278 0.6900699328 -1.2163755537
H 3.8728005861 1.1085722448 0.4701739634
H 3.7786294629 2.4214409231 -0.754036784
H -0.055179539 -2.1717301299 0.4646426166
H 1.1735191565 -2.5012875913 1.7091156259
H 1.352429479 -3.2028021411 0.1068101746
H -2.7319301626 1.1174175175 1.5441596964
H -2.861318573 -0.3161767867 0.5218716926
H -2.1462498291 2.5005882683 -0.4591459174
H -3.7243887533 1.723088777 -0.7033245422
H 0.760103308 0.5472383495 1.9305928031
H -1.0569363427 -0.383642113 -3.491597846
H 0.1808513084 2.5594182914 3.2314281722
H -1.3970510657 2.6718248249 2.4475466357
H 0.0933691563 2.8692564692 1.4826975308
H -0.3191170952 0.1661329796 4.1019998287
H -0.7983390436 -1.1014185318 2.9598710785
H -1.9292111243 0.2026646876 3.3833876037
H 0.8571232718 0.4927768503 -4.5762887316
H 1.7339355845 0.759799285 -3.0581959093
H 0.338945638 1.7654915635 -3.4466152562
H -2.808963694 0.0236138627 -2.1237249084
H -2.0117206926 1.5119746961 -2.6509122837
H -0.1968916127 -2.37445145 -2.2429319983
H 1.4299267186 -1.6586837308 -2.2861968071
H 0.5870718915 -2.0412211501 -3.7951640089

3-SCRF

B3LYP/6-31G(d) energy (a.u.): -847.214254

C 2.061462383 1.2556510685 -0.4749425954
C 1.2910656655 0.0648796762 -0.2445972216
C 3.5792574371 1.219317497 -0.3896935859
C 0.8500973871 -2.3199922633 0.5769883553
C 1.8192998962 -1.1964339748 0.1875638178
O 1.5070435587 2.3497260185 -0.7432252458
O 3.037447617 -1.4546256273 0.296769259
C -0.177943454 0.2680199979 -0.3696888866
N -0.8963857231 0.5694786965 0.7327810236
C -2.3544048651 0.7679381861 0.6712258069
N -0.7888127998 0.1474570986 -1.56149363
C -2.7251734716 1.4126267722 -0.6521425542
C -0.2536820561 0.8524259353 2.0472150295
C -0.1488287062 -0.2564335637 -2.8621516262
C -0.2174187136 2.3623666326 2.3207953559
C -0.9225304034 0.0583187932 3.1762700708
C 0.5035314595 0.9421019642 -3.5620567199
C -2.2049427962 0.5336174107 -1.7710645009
C 0.7541275668 -1.4935407881 -2.8360908042
H 4.002467429 0.5268258245 -1.1250912867
H 3.9190202036 0.858560502 0.5853949178
H 3.9532385038 2.2310740751 -0.5724782755
H -0.1880575831 -2.1703421843 0.2688132676
H 0.8700669413 -2.4382293756 1.6681806644
H 1.2146049089 -3.259823456 0.1492221629
H -2.6531317436 1.4000024594 1.5087522218
H -2.8609181259 -0.1996633332 0.7886728919
H -2.2820374761 2.4135371153 -0.7132350794
H -3.8117191641 1.5155724787 -0.7384825593
H 0.7728136134 0.5057792049 1.9497976486
H -1.0190188505 -0.5501598563 -3.4616487882
H 0.3419460207 2.5517406363 3.2439779579
H -1.2207532426 2.7848147128 2.4522121378
H 0.2814534377 2.8784476637 1.4958260868
H -0.3456856037 0.1982204152 4.0967658533
H -0.9469046542 -1.012745151 2.9498751428
H -1.9461772661 0.3929343733 3.3775102012
H 0.823781874 0.6417998868 -4.5662198201
H 1.3677883438 1.3105836516 -3.0084935124
H -0.2052332773 1.7708555179 -3.6687625979
H -2.803165427 -0.3829835803 -1.8607659541
H -2.2645785653 1.0602413289 -2.7285660881
H 0.3014883349 -2.3065481701 -2.2607209689
H 1.7481202522 -1.2896684041 -2.437834773
H 0.8642551346 -1.8405638657 -3.8703657993

3·2H₂O

B3LYP/6-31G(d) energy (a.u.): -1000.0537832

C 1.2050865483 0.4822733576 -0.5003197478
C 0.4095370004 -0.6961214798 -0.2811408442
C 2.7196469045 0.4058305854 -0.5153032242
C -0.0263677951 -3.1283930524 0.4180121415
C 0.9316040578 -1.9783998743 0.0902740613
O 0.6838415942 1.6156928878 -0.6491760351
O 2.151110855 -2.2424494472 0.1863619918
C -1.0466739921 -0.4315453058 -0.1799885602
N -1.5841368055 -0.2344295943 1.0416836663
C -3.0363312335 -0.0701234301 1.1908821965

N -1.8312353545 -0.3887858846 -1.2718984266
C -3.5610824589 0.813481913 0.0704049029
C -0.7486483726 0.0084159627 2.2577445615
C -1.4177455622 -0.7765348798 -2.6646411164
C -0.7618028846 1.4973263604 2.6295315967
C -1.1720990742 -0.9009216429 3.416156981
C -0.5510307307 0.2800576843 -3.3610900701
C -3.2063041547 0.1675833381 -1.2562757879
C -0.8536661738 -2.1945510222 -2.7989360983
H 3.0893639231 -0.3908630388 -1.1650646988
H 3.0796408097 0.1678173901 0.4909284909
H 3.1038318554 1.3805804052 -0.8265761277
H -1.0839063116 -2.9241773235 0.2299072363
H 0.0981244499 -3.3925573444 1.4747861269
H 0.2761838056 -4.0040781174 -0.1652298984
H -3.2341700783 0.3691851065 2.1684223351
H -3.5153301102 -1.059220238 1.1702441234
H -3.1009616871 1.8043753268 0.1232559315
H -4.647821837 0.9304963583 0.1421473027
H 0.2711959736 -0.2576168517 1.9914688817
H -2.3806885971 -0.7892289542 -3.1863327263
H -0.0747231387 1.662290945 3.4664175113
H -1.7542464578 1.8444691364 2.943659392
H -0.4265526563 2.1015478384 1.781937622
H -0.4226615421 -0.8225807164 4.2093313487
H -1.2151368648 -1.948538535 3.1018307128
H -2.1441818458 -0.6250003074 3.8424256701
H -0.5636851332 0.0894790823 -4.4407107851
H 0.4844227615 0.2365310962 -3.0197751357
H -0.9320399836 1.2874302868 -3.1729594436
H -3.9002753184 -0.6486246336 -1.4986142463
H -3.2576235576 0.9156696774 -2.0518536995
H -1.4698234562 -2.9233368604 -2.2624928771
H 0.1733058379 -2.2676393042 -2.4396977107
H -0.8611558844 -2.4658730855 -3.8609782877
O 2.4863602875 -1.1780860649 2.7736751925
H 3.3745038953 -0.806415737 2.8768124487
H 2.5307418812 -1.667351474 1.924621383
O -1.6425357597 2.8968519381 -1.3847971709
H -0.8442241221 2.400000018 -1.0875307405
H -1.2985695067 3.7761935046 -1.5996103499

3·H₂O-SCRF

B3LYP/6-31G(d) energy (a.u.): -1000.0759687

C -0.9892320488 -0.7263161007 1.3420543123
C -0.7921427693 -0.42592647 -0.0490157363
C -2.2976326151 -1.3136848664 1.8370493343
C -1.486381332 0.0116124658 -2.4756486929
C -1.8122488428 -0.4510821084 -1.0533520934
O -0.0952961973 -0.5078225688 2.2004004808
O -2.9949258196 -0.8275664855 -0.8683794974
C 0.5628359457 0.0976305984 -0.381083118
N 0.7573725086 1.4312100207 -0.4433335679
C 2.0555479138 1.9696287785 -0.8830056227
N 1.5817007319 -0.7402906109 -0.631883448
C 3.173245303 1.1510254615 -0.2583088575
C -0.2295072105 2.4093560323 0.0951514232
C 1.4833098839 -2.234319832 -0.793155817
C 0.2507553198 2.9786686721 1.4375392712

C -0.5523927125 3.4999323332 -0.9331410645
C 1.2943217632 -2.9767529336 0.535490972
C 2.9985420408 -0.2947093034 -0.6828403994
C 0.5188774801 -2.7086503203 -1.884419967
H -2.5987488359 -2.1833130425 1.2458543075
H -3.1198176796 -0.5959687265 1.7531221797
H -2.1651577533 -1.5939159713 2.8858507293
H -0.4279523609 0.1882375363 -2.6785071674
H -2.0372974682 0.9386728171 -2.677339032
H -1.8598915588 -0.7402931897 -3.1784792649
H 2.1164201232 3.0168188298 -0.5863221153
H 2.1065664076 1.9306483175 -1.9797241419
H 3.1303394087 1.2263231489 0.8322558371
H 4.1511204652 1.5139527157 -0.5924618686
H -1.1361308955 1.8361229573 0.2784132079
H 2.4848973364 -2.4871836996 -1.1569837602
H -0.5298002319 3.6219963419 1.858979665
H 1.1557646096 3.5880998353 1.3297732014
H 0.4506810428 2.1654125341 2.1407954883
H -1.3589128092 4.1300069199 -0.5429353294
H -0.8865584591 3.0660515912 -1.8809596797
H 0.3040427293 4.1527872599 -1.1347866059
H 1.5800707725 -4.0257646569 0.3958450163
H 0.2543967275 -2.9508475679 0.8668968116
H 1.9183899473 -2.5403552931 1.3203523841
H 3.3605054008 -0.4526272504 -1.7067380495
H 3.561466373 -0.9514800581 -0.0134882411
H 0.6551403275 -2.1432157312 -2.8117290493
H -0.5262657945 -2.6458715896 -1.5782366827
H 0.743363121 -3.7599917436 -2.0983422814
O -5.3088439486 -0.1767913385 0.5994893111
H -4.4984332785 -0.4374752737 0.113590576
H -5.3131861926 0.7956197248 0.5196450264
O 2.6767007555 -0.4447106908 2.5668798431
H 1.7159959764 -0.4055396237 2.3648806264
H 2.7009019911 -0.8012866929 3.4755354462

5

B3LYP/6-31G(d) energy (a.u.): -1447.461 7031

C 0.4602591643 1.0600927286 -0.4078469537
C -0.3013933414 -0.1971807655 -0.2551274026
O 1.8012869216 0.9244952509 -0.6455143407
C 2.4353863626 -0.3458832815 -0.4583272834
O 1.6505089155 -1.384096464 -1.0530981087
C 0.302730014 -1.4126622207 -0.8333178461
C 2.6552845482 -0.6258939756 1.0289074761
C 3.7306436033 -0.2898460104 -1.2506197021
O -0.0032023369 2.180910262 -0.4250008465
O -0.3073435536 -2.4133156078 -1.1508738013
C -1.6216578256 -0.2278517973 0.1892951847
S -2.644761624 -1.6229659424 -0.1801666863
C -4.2229227373 -1.2861460274 0.6894940883
S -2.4162848082 1.0297251046 1.1282372727
C -1.1394726991 1.8636695913 2.1314684291
H 3.1734057894 -1.5811883856 1.1520045411
H 1.7040923055 -0.6772461179 1.5664223445
H 3.2644834903 0.1687407378 1.4692458016
H 4.2566812687 -1.2451612315 -1.1731166552
H 4.3707975553 0.5073424013 -0.8631049038

H 3.5066996359 -0.0891914466 -2.3011047408
H -4.8146195783 -2.1845471947 0.4895207609
H -4.7518411702 -0.4199497652 0.2864378995
H -4.0863187642 -1.1752771228 1.7668956397
H -0.6736042142 2.6758268853 1.5765861886
H -0.3855097334 1.1420077999 2.4547230962
H -1.6789381882 2.2368655949 3.0061155481

5-SCRF

B3LYP/6-31G(d) energy (a.u.): -1447.4767062

C 0.4436174091 1.05551534 -0.4485636424
C -0.3124169132 -0.1981118779 -0.2808195436
O 1.7833962366 0.9303534083 -0.6730109042
C 2.4312950216 -0.3338728835 -0.4551347903
O 1.6472224024 -1.3801296142 -1.0521311773
C 0.300452416 -1.405983821 -0.8526600524
C 2.6303834608 -0.593857977 1.0355099648
C 3.7330910659 -0.2818522745 -1.2338102482
O -0.0265300642 2.1779711015 -0.496333689
O -0.2991669604 -2.4133490239 -1.1896366838
C -1.632979103 -0.2239497188 0.1762292085
S -2.6743556345 -1.5955995659 -0.206803375
C -4.2335681731 -1.2873115555 0.7015157602
S -2.3976315817 1.0217272026 1.1478990672
C -1.0922596731 1.8192045736 2.1447748626
H 3.1618264926 -1.5397656948 1.1745136586
H 1.6746805603 -0.6529277311 1.5639314245
H 3.2254239992 0.2129502226 1.4731248936
H 4.26249046 -1.2335532265 -1.1352628266
H 4.3664252717 0.5197546862 -0.8437346016
H 3.5246254996 -0.0935508428 -2.2903762321
H -4.8264396794 -2.1830376906 0.4924463224
H -4.7682102593 -0.4118898238 0.3273098166
H -4.0669709449 -1.2036657822 1.7773010451
H -0.609494561 2.6247736411 1.594735412
H -0.3595308858 1.0756918438 2.4667802378
H -1.6209868625 2.2057400844 3.0203410926

6

B3LYP/6-31G(d) energy (a.u.): -1008.8878068

C 1.2624315208 0.6635704558 0.2369619003
C 0.4624287096 -0.5573242477 0.2334808243
O 2.6047874586 0.5121790932 0.0008430551
C 3.2062444636 -0.7820458492 0.1377907908
O 2.3985902227 -1.8009851299 -0.4519261879
C 1.0433273786 -1.8278396497 -0.2023653673
C 3.4464246945 -1.0922072644 1.6168520682
C 4.4910103312 -0.7358492157 -0.6735170526
O 0.8330160846 1.7985697502 0.3557529924
O 0.4571421369 -2.8773567111 -0.3709056309
C -0.9220999913 -0.4748295348 0.5108489962
N -1.4349510997 0.3051998187 1.4935800106
C -2.7908507013 0.8502865501 1.4385559182
N -1.8593816595 -1.2140560575 -0.1731899234
C -1.8380518633 -1.616788116 -1.5215244608
C -2.5519842975 -2.7565546166 -1.9024351667
C -2.5960007175 -3.0954926084 -3.2522561172
N -1.9920803284 -2.3992440338 -4.2225595507

C -1.312924787 -1.3102637439 -3.8375370672
C -1.2093454343 -0.8668401979 -2.5217785636
C -0.6333678593 0.7900455153 2.6113077649
H 3.9436315135 -2.0613240617 1.7164459793
H 2.5002222704 -1.132765155 2.1647353595
H 4.0767264253 -0.3177881264 2.0635853036
H 4.9993183082 -1.7026590859 -0.6239947485
H 5.1534429614 0.0411498365 -0.2820610984
H 4.2545597767 -0.5105996791 -1.7164355688
H -2.7472818878 1.9266975918 1.638165273
H -3.4413167151 0.386347918 2.1918140298
H -3.2184466786 0.697486851 0.4476223747
H -2.6233185529 -1.5881085845 0.375887697
H -3.0456270658 -3.3790869142 -1.1610785305
H -3.1447518281 -3.9814735484 -3.5674415523
H -0.8292204607 -0.7441115194 -4.6316976431
H -0.6611522442 0.0380885294 -2.2859104
H -0.2532616816 1.7962979084 2.4110656763
H 0.2128136495 0.1197815066 2.7689492481
H -1.2594900523 0.7925043263 3.5100563675

6-SCRF

B3LYP/6-31G(d) energy (a.u.): -1008.9183364

C -1.5830083784 0.4021810292 0.9967849549
C -0.6592073899 0.35831499 -0.1173656237
O -2.4946522818 -0.6204552829 1.085156858
C -2.7594828142 -1.4312786397 -0.0709966254
O -1.5398214716 -1.7855403205 -0.7333306541
C -0.5846745755 -0.8175009867 -0.9636734641
C -3.6868209323 -0.6889200449 -1.0323730465
C -3.3570261659 -2.7281165478 0.4481692378
O -1.5780753327 1.2177482132 1.9111303789
O 0.2316115726 -1.0479855258 -1.8423278061
C 0.2948380409 1.4132481204 -0.2756799196
N -0.0449986725 2.7081379139 -0.1756198817
C 0.9221829558 3.7597771896 0.1531826452
N 1.6129041679 1.1596799906 -0.5670840308
C 2.3595383518 0.0490008366 -0.137131845
C 3.4122242934 -0.4233023045 -0.9282984295
C 4.1839486867 -1.4795042756 -0.4530326812
N 3.9810397731 -2.0909737115 0.7249216096
C 2.9709636107 -1.6188099472 1.47464083
C 2.1460490023 -0.559583366 1.1072856701
C -1.4225885386 3.1763231394 -0.3108834624
H -3.921721709 -1.3290157394 -1.8879333633
H -3.2182237071 0.2270531491 -1.403842813
H -4.6174132405 -0.4246163191 -0.5215992776
H -3.5683874613 -3.4022279467 -0.3866766191
H -4.2884508871 -2.5222574102 0.9832292637
H -2.6519357203 -3.2119947917 1.1296540584
H 0.4756599671 4.4156165855 0.9073168147
H 1.1681134213 4.3592417443 -0.7315217486
H 1.8335388889 3.3179043305 0.5566158921
H 2.0597448239 1.7444174957 -1.2797274053
H 3.6209316567 0.0212939168 -1.9000546797
H 5.007362259 -1.8589907089 -1.0597156825
H 2.8170376741 -2.105961043 2.438529074
H 1.3736152944 -0.2115834483 1.7856176372
H -1.8807507624 3.3111887985 0.6734314927

H -2.0030172338 2.4505264924 -0.8808371195
H -1.4108708795 4.1285554572 -0.8496444817

7

B3LYP/6-31G(d) energy (a.u.): -1312.4012924

C 1.5797955633 0.5115122988 -0.8238872259
C 0.7043561235 -0.4505150403 -0.1281163765
O 2.8954566452 0.1378851194 -0.9188884241
C 3.4142498604 -0.8610789655 -0.0316839736
O 2.5502520736 -2.0047902211 0.0045527046
C 1.2011395433 -1.8256932839 0.1181488456
C 3.5922791614 -0.2861725131 1.3734443789
C 4.7162535133 -1.3375225962 -0.6525234464
O 1.2433710121 1.5756229522 -1.2951398788
O 0.5033274582 -2.7982440151 0.3039343215
C -0.5709728692 -0.0896064888 0.2836115469
S -1.2684788883 -0.7776047836 1.7869441573
C -2.6715063982 -1.7542101672 1.1195497612
N -1.353251349 0.8784187283 -0.2698189944
C -1.5316234341 1.2771131593 -1.6122971587
C -2.2753381612 2.4372527488 -1.8530216152
C -2.543287424 2.7964349249 -3.1714550461
N -2.1388689493 2.0944547657 -4.2361605966
C -1.4326147978 0.9840544632 -3.9843114043
C -1.0996677774 0.5291569114 -2.7116345659
H 4.0113140222 -1.0500227064 2.034587152
H 2.6357684868 0.0440795447 1.7890526438
H 4.2719429491 0.5699923009 1.3398263006
H 5.1553161791 -2.1271002762 -0.0368504003
H 5.4201227085 -0.5043743326 -0.7275268167
H 4.5215857987 -1.7319442185 -1.6529118576
H -3.2689542474 -2.0635127473 1.9807605364
H -2.2724369038 -2.6316957647 0.6078503733
H -3.2926678283 -1.1588682019 0.4463021893
H -2.0313682959 1.2731767882 0.373001512
H -2.6293536414 3.0541756403 -1.0309492013
H -3.1150022004 3.6993190105 -3.3788310579
H -1.1102856991 0.4159690605 -4.8549474944
H -0.5309072339 -0.3840090947 -2.5873308884

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B3LYP/6-31G(d) energy (a.u.): -1312.429139

C 1.5152316406 0.5885207564 -0.6714572743
C 0.7061736778 -0.5184749619 -0.1511223774
O 2.854274632 0.329157444 -0.8171307518
C 3.4482298702 -0.7496628628 -0.0802869689
O 2.6555147177 -1.9384751679 -0.2302735032
C 1.2968485649 -1.8653970968 -0.0988080994
C 3.5845473376 -0.3818015632 1.3957142709
C 4.7797282323 -1.0391195364 -0.7496864191
O 1.1221303283 1.6977095824 -0.9836489785
O 0.6853221721 -2.9169456241 -0.0491063967
C -0.6171600871 -0.2871026986 0.2622747558
S -1.2180808455 -1.1443617046 1.6810504465
C -2.988349351 -1.4431311387 1.3047642945
N -1.4448582187 0.6423718407 -0.2761281725
C -1.5254958749 1.0733302188 -1.6193704184
C -2.1142934253 2.3120804834 -1.8892808783

C -2.2712960207 2.6996500859 -3.2172951089
N -1.8921878508 1.9548410409 -4.2669220289
C -1.3395437026 0.7629038115 -3.9857778269
C -1.1390736242 0.2711131558 -2.6994313307
H 4.0584597631 -1.205328713 1.9377117741
H 2.609318862 -0.1815391862 1.8490428757
H 4.2067140241 0.5122539518 1.4964652412
H 5.2710775075 -1.8789961644 -0.2507419373
H 5.4267996764 -0.1599167804 -0.6860044421
H 4.6180972783 -1.2909853286 -1.8012750249
H -3.3176109074 -2.1743367874 2.0478306921
H -3.0925945898 -1.8716421745 0.30590726
H -3.5925431688 -0.5388917886 1.4029787321
H -2.089798055 1.1144417777 0.3674806754
H -2.4397980222 2.9645260001 -1.0801149712
H -2.7247671436 3.6650476169 -3.4455575357
H -1.0453091427 0.1537220365 -4.8413482774
H -0.7057632545 -0.7139075248 -2.5571722957

8

B3LYP/6-31G(d) energy (a.u.): -1312.4028308

C 0.5811072299 -0.3103577525 0.9487000933
C -0.245927201 -1.5202322533 0.8474055483
O 1.9272283198 -0.4829165791 0.7165290224
C 2.4902125063 -1.7955935141 0.7621666116
O 1.6829801622 -2.7185136351 0.0261228697
C 0.3292694734 -2.7243841142 0.2502246927
C 2.6413914552 -2.2600006694 2.2120871538
C 3.8164283042 -1.7129877198 0.0237921265
O 0.2003889866 0.8230507169 1.1640304188
O -0.2990236141 -3.7064485148 -0.0985773655
C -1.5782203835 -1.5265792916 1.2958972223
S -2.5631978038 -3.0110354998 1.1346461271
C -4.0732793406 -2.5091479514 2.0422582548
N -2.1634930144 -0.5296337985 1.9838904469
C -2.5663946618 0.6309905258 1.5457623809
C -3.0835218679 1.604456745 2.4825708186
C -3.5423000451 2.810295291 2.0610902306
N -3.5449386989 3.1386716247 0.7289109962
C -3.0707306012 2.2549074247 -0.2072591693
C -2.5931185082 1.0375388158 0.1540378202
H 3.092717802 -3.2561373869 2.2378116002
H 1.6694291567 -2.3051099265 2.7115556452
H 3.2821733224 -1.5624755217 2.759514693
H 4.2936751676 -2.6965860479 0.001239427
H 4.479006306 -1.0015320993 0.5243182894
H 3.6419784046 -1.3776242952 -1.0016861466
H -4.6965769028 -3.4083191515 2.0577356936
H -4.6135597986 -1.7081225101 1.5334092703
H -3.8413491088 -2.2021352007 3.0635843592
H -3.0832434853 1.3589815623 3.5378885199
H -3.924070035 3.5670013829 2.736713467
H -3.8736541483 4.047222749 0.4374878598
H -3.0959400531 2.5967351343 -1.235739771
H -2.2113963244 0.3641744607 -0.603628207

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B3LYP/6-31G(d) energy (a.u.): -1312.4400432

C -0.8918952614 -1.1428321202 0.1921791754
C -0.8961156506 0.2881716462 -0.0946123711
O -2.1067015195 -1.7896143986 0.0945508262
C -3.3180366817 -1.0332113949 0.1610174155
O -3.2275005684 0.1128014707 -0.6976604547
C -2.1001793712 0.8905043619 -0.6393898423
C -3.5976944406 -0.5954109188 1.5983111386
C -4.4103733242 -1.9158955792 -0.4173545212
O 0.0659403238 -1.8433096178 0.4748670864
O -2.19529419 2.0224673509 -1.0992613752
C 0.2637650641 1.0787262011 0.1508350729
S 0.1714445465 2.8620246166 -0.1069234957
C 1.8159949494 3.3769391085 0.5041117503
N 1.3944383192 0.6625699295 0.6856639024
C 2.3159716302 -0.1859132707 0.2655584041
C 3.3382465013 -0.62892963 1.170789987
C 4.3433737382 -1.4475821532 0.7423375689
N 4.4055464455 -1.8541248742 -0.5565100556
C 3.4678278549 -1.4576409198 -1.4610527749
C 2.4332148621 -0.6463591578 -1.0923028528
H -4.5340810165 -0.0310551032 1.6386876933
H -2.7911618455 0.0366651142 1.9815879849
H -3.6876130442 -1.4758776185 2.2414842486
H -5.3635545451 -1.3796173917 -0.4162382712
H -4.5127196876 -2.8236890808 0.1838869614
H -4.1561690866 -2.1930560419 -1.4441669473
H 1.8131828997 4.4685287388 0.4265224557
H 2.6195828097 2.9714921031 -0.1132161182
H 1.964893066 3.0781994903 1.5432296062
H 3.3050903932 -0.309744587 2.2088061956
H 5.1331418668 -1.8112734496 1.3948779631
H 5.1727802347 -2.4662889784 -0.8593090197
H 3.5969272285 -1.8296911753 -2.4745990978
H 1.6994699286 -0.3462416164 -1.8346314973

8

MP2/6-31G(d) energy (a.u.): -1309.1085883

C 0.6202026801 -0.2537779331 0.8774851618
C -0.2098909871 -1.4617121075 0.7581254417
O 1.9728909739 -0.4488019508 0.6925672149
C 2.466998329 -1.7908112467 0.7549768553
O 1.7013015319 -2.6502861669 -0.0980577469
C 0.33663476 -2.6357468325 0.0783078183
C 2.4536117567 -2.3027581095 2.1860484785
C 3.8495880474 -1.7448345729 0.1506767825
O 0.2288628756 0.8861930967 1.0651372314
O -0.3199627679 -3.5674965001 -0.3624821376
C -1.502756509 -1.4833409309 1.2665357239
S -2.5392410136 -2.8974427629 1.0532428403
C -3.9448372975 -2.4008437244 2.0844676563
N -2.0062813905 -0.5039543138 2.069291777
C -2.501956657 0.6127890184 1.5943166797
C -2.9943470606 1.6078161208 2.5112786848
C -3.5327516159 2.7757338778 2.0625816592
N -3.6328319671 3.0301284251 0.7192854713
C -3.1775841875 2.1226837256 -0.2002979682
C -2.6235657662 0.9419665125 0.1936756806
H 2.8574176327 -3.3178626933 2.2124111788
H 1.4375489137 -2.315502382 2.5864811592

H 3.0702934327 -1.6505086422 2.8093738888
H 4.2807778434 -2.748168812 0.1397403407
H 4.4858233907 -1.0776654022 0.7361750842
H 3.7761829166 -1.3707500718 -0.8718246805
H -4.6161154977 -3.26376464 2.0799295898
H -4.4708272501 -1.5390460571 1.6726419153
H -3.6323192674 -2.1831288813 3.1054812
H -2.9138971337 1.4189982502 3.5765761546
H -3.903941611 3.5505562661 2.7250160914
H -4.0197994472 3.9102747819 0.4036535192
H -3.2771105556 2.4091887638 -1.2422340787
H -2.2540661016 0.2500288949 -0.5560936677

8

MP2/6-311++G(d,p) energy (a.u.): -1309.6406145

C -0.923514 -1.240591 0.082557
C -0.884252 0.212164 -0.167578
O -2.179716 -1.798981 0.063791
C -3.291661 -0.913047 0.193879
O -3.207688 0.129677 -0.779261
C -2.048117 0.861277 -0.782529
C -3.365603 -0.335232 1.601361
C -4.512603 -1.724788 -0.17512
O 0.028089 -1.97444 0.243726
O -2.041613 1.952775 -1.313742
C 0.217288 0.968017 0.223509
S 0.299849 2.693727 -0.108028
C 1.836067 3.099054 0.763063
N 1.239155 0.458481 0.970883
C 2.209252 -0.212222 0.399638
C 3.253463 -0.787083 1.212407
C 4.272358 -1.497236 0.647211
N 4.35167 -1.656203 -0.711921
C 3.39642 -1.121449 -1.533098
C 2.354096 -0.401612 -1.025949
H -4.240251 0.315997 1.677651
H -2.470576 0.244936 1.840589
H -3.45762 -1.153254 2.32043
H -5.401075 -1.091056 -0.126386
H -4.618674 -2.560757 0.519952
H -4.394654 -2.108749 -1.190341
H 1.949707 4.179329 0.636089
H 2.695267 2.595756 0.317668
H 1.769666 2.85471 1.823278
H 3.199981 -0.679708 2.290357
H 5.063012 -1.960506 1.22791
H 5.095641 -2.213837 -1.107409
H 3.526505 -1.301154 -2.595093
H 1.605724 -0.002736 -1.703629

9

B3LYP/6-31G(d) energy (a.u.): -1311.8806399

C 2.5541945415 3.3167443601 -1.1626008283
C 1.8426891647 2.11060372 -0.8609720492
O 3.9240867178 3.1511300647 -1.4303242639
C 4.5506386269 1.9578518879 -0.978412229
O 3.7976098752 0.7962163885 -1.3138093681
C 2.4194136461 0.8163742545 -1.0617179167
C 4.7846736249 2.0182299592 0.5383842755

C 5.8565866338 1.8485975595 -1.7579702099
O 2.1203212419 4.4568776605 -1.2266171548
O 1.8420358695 -0.2624407369 -1.1081360721
C 0.4172252775 2.2111868598 -0.5173382289
S 0.0388670275 1.5962536796 1.125303406
C -1.7861113331 1.6512860244 1.1333455935
N -0.5454638811 2.7392042455 -1.1838401167
C -0.4166947584 3.0656425647 -2.5314987209
C -0.7959189653 4.3364284066 -2.9937938663
C -0.7894780162 4.5895698795 -4.3605873642
N -0.4538850208 3.6926086347 -5.3017737726
C -0.0894456791 2.4827298977 -4.847148974
C -0.0495635675 2.1178134686 -3.5052853197
H 5.2986581438 1.1115972259 0.875237081
H 3.8297850796 2.0953762868 1.0639014427
H 5.3961378537 2.8917591469 0.7884975499
H 6.392863347 0.9378821955 -1.4725112909
H 6.4898327176 2.7188226146 -1.5583150832
H 5.6332535067 1.8095270278 -2.8275377319
H -2.1128146514 1.2676214339 2.1050918974
H -2.1879558316 1.0256631158 0.3325936326
H -2.1408323684 2.6742999286 0.9925990724
H -1.0752004697 5.1045755557 -2.2799845869
H -1.0768015929 5.5762098048 -4.7270075488
H 0.1884219098 1.7537924887 -5.609586711
H 0.2514683298 1.1198663962 -3.2010265427

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B3LYP/6-31G(d) energy (a.u.): -1311.9644888

C 2.5184773346 3.3329438543 -1.0695423061
C 1.8056059647 2.1222504221 -0.8340127048
O 3.8719529343 3.1957397182 -1.3724839204
C 4.5295169943 1.9809732211 -0.9987016632
O 3.7495549843 0.8375901794 -1.3723735093
C 2.3897666857 0.8499725596 -1.0871687506
C 4.8028180929 1.9631639031 0.5077471386
C 5.8049930515 1.9139183989 -1.82473983
O 2.076742337 4.4810937172 -1.0622802536
O 1.813056666 -0.2386011254 -1.1502689943
C 0.3669201271 2.2031200005 -0.5032022459
S 0.003565457 1.6312431633 1.1518232199
C -1.8206979905 1.6969123738 1.213473738
N -0.5932561045 2.6767782793 -1.2093510163
C -0.4161640058 3.0115796368 -2.5547254026
C -0.768793202 4.2901655146 -3.0150679395
C -0.688556004 4.5642818257 -4.3763768297
N -0.3042400729 3.6726798712 -5.3075489213
C 0.0215177613 2.4485692966 -4.8566931716
C -0.0130523064 2.0696766976 -3.5179927811
H 5.3361381604 1.0464042423 0.7776809308
H 3.8674614875 2.0045626921 1.0720252039
H 5.4191014577 2.8243648998 0.7840659295
H 6.3455293184 0.9880288654 -1.6066893971
H 6.4506884622 2.7650022005 -1.5889760914
H 5.5560165346 1.9393508774 -2.8894983095
H -2.1121641798 1.3566574651 2.2108974912
H -2.2510481108 1.0385610172 0.4554417118
H -2.1716006813 2.7173361493 1.0482709243
H -1.093531823 5.0525782621 -2.3108984079

H -0.9532118503 5.5574815681 -4.7436681359
H 0.329331639 1.7245968766 -5.6135058354
H 0.2561578809 1.0609253762 -3.2185018709

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MP2/6-31G(d) energy (a.u.): -1308.6021109
C 2.4486346179 3.3470486211 -1.1639299322
C 1.7821606885 2.1264076781 -0.8483020948
O 3.810845069 3.2090572098 -1.4968044398
C 4.4428359489 2.00732071 -1.0688919938
O 3.7097299412 0.8456123516 -1.4535317303
C 2.3392718839 0.8509753403 -1.1478776708
C 4.6637065087 2.0230370445 0.4401024995
C 5.7424323086 1.9371182108 -1.8429373942
O 1.98142071 4.483950445 -1.1947144472
O 1.7481044159 -0.2274600522 -1.2351840762
C 0.3764055574 2.2015627651 -0.4539578281
S 0.0616999513 1.5977874415 1.1776799646
C -1.7453418347 1.6378738892 1.1999054695
N -0.6129241791 2.7120567954 -1.1186926401
C -0.3715164357 3.0269501114 -2.4664071189
C -0.6510055045 4.3074054499 -2.9535258137
C -0.528867967 4.5488995139 -4.3192430629
N -0.1695622487 3.6205178885 -5.2280270278
C 0.0992657735 2.3938691924 -4.7366249558
C 0.0149866576 2.045770312 -3.3903225059
H 5.1892148316 1.1124374027 0.7421347941
H 3.7037231111 2.0704226642 0.9563393977
H 5.2622641438 2.8971681365 0.7124058669
H 6.2821376521 1.0227044933 -1.5830774259
H 6.3606346579 2.8085073955 -1.6120002705
H 5.5109954145 1.9304453294 -2.9096720088
H -2.0695488059 1.1958309063 2.1460574693
H -2.141174221 1.0595631953 0.3636619187
H -2.1125178805 2.6613763824 1.1193532348
H -0.9330316026 5.0952346403 -2.2613714688
H -0.733261338 5.5434084928 -4.7168347087
H 0.398384644 1.6467021137 -5.472054793
H 0.2484945302 1.0403399295 -3.0464972067

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MP2/6-311++G(d,p) energy (a.u.): -1309.1404809

C 2.408707274 3.3209224956 -1.1671156437
C 1.7506616858 2.0920932326 -0.8561911632
O 3.7534571469 3.1943762496 -1.5433217718
C 4.4033473378 2.0084718507 -1.1101185375
O 3.6834504163 0.8424084135 -1.4908931842
C 2.3283957449 0.8203128237 -1.1411981837
C 4.630151838 2.0352742744 0.4016137425
C 5.7089666303 1.9511607835 -1.8795527052
O 1.9310853437 4.4480646043 -1.1650584741
O 1.7613815356 -0.266664807 -1.1834053225
C 0.3436392703 2.1629519698 -0.4490186756
S 0.0501604524 1.5863754581 1.1874252431
C -1.7535559555 1.6609489987 1.2445859081
N -0.6420642284 2.6711103298 -1.1212640805
C -0.3756384226 3.0002230249 -2.4617156438
C -0.6555433945 4.285735889 -2.9420801061
C -0.4702577096 4.5570819506 -4.2994534067

N -0.0442401587 3.655028218 -5.205373474
C 0.2189475461 2.4224814847 -4.7264342473
C 0.0754252175 2.0459338307 -3.3883730039
H 5.1606791829 1.1267361301 0.7024362415
H 3.6782252486 2.0863944208 0.9343639719
H 5.2323689614 2.9117110024 0.6596165395
H 6.2574074166 1.0450275831 -1.6076992949
H 6.3128793923 2.8323467322 -1.6462273508
H 5.4874813684 1.9352035316 -2.9488724708
H -2.0562392053 1.2903422845 2.2282048887
H -2.1825802998 1.0315292417 0.4623277788
H -2.0998546288 2.6861037599 1.1065356015
H -0.9855653217 5.0576174099 -2.2531438569
H -0.6728948303 5.5561110142 -4.6840181093
H 0.5694770304 1.6938351805 -5.4563829186
H 0.3007351152 1.0326526339 -3.0630402905

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B3LYP/6-31G(d) energy (a.u.): -1104.6567126

C 0.2666693145 1.4256557353 0.2242039629
C -0.5282119333 0.2037147008 0.2187293179
O 1.6044838091 1.3140858347 -0.0127860869
C 2.2659437741 0.0759722992 0.2933557532
O 1.5008894821 -1.029252131 -0.1897174733
C 0.1409824199 -1.0745199668 0.018719387
C 2.4643443293 -0.0416574754 1.8034994329
C 3.5674862439 0.0805182708 -0.4880980284
O -0.163234162 2.5692095194 0.3760609019
O -0.366287477 -2.1845107018 -0.0101138682
C -1.9361842778 0.2992823683 0.4412143482
S -3.1335240342 -0.9751497051 0.1009624999
C -2.7199502552 -1.5639352656 -1.5831722144
N -2.4656890215 1.4047262003 0.9629978084
C -3.8791952474 1.7247876259 1.1436677639
H 2.9883122856 -0.9734491187 2.0354952697
H 1.5024987828 -0.0430397531 2.326478155
H 3.0592786005 0.8008269765 2.1681745378
H 4.1136078267 -0.8490587176 -0.3050523697
H 4.187867326 0.9248390828 -0.1745806006
H 3.3561530503 0.1676817076 -1.5574104127
H -3.6408188998 -2.0301881653 -1.9441916773
H -1.9060588161 -2.2845947951 -1.5497105292
H -2.4714223412 -0.7170812582 -2.2256273429
H -1.7865334511 2.1441876448 1.1535392513
H -4.3206120272 1.1427737353 1.9592428921
H -4.4432329107 1.5301924765 0.227397031
H -3.9427373905 2.7852308758 1.3954282905

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B3LYP/6-31G(d) energy (a.u.): -1104.6567119

C 0.7189930214 1.252691305 -0.4648900932
C -0.1010933478 0.1293239905 -0.0299268621
O 2.0491368859 1.028120596 -0.6629354371
C 2.6914279446 -0.0364276563 0.0568547376
O 1.8937366963 -1.220781294 0.0122183486
C 0.5374135527 -1.1522437901 0.2364890345
C 2.921086878 0.3876217981 1.506351348
C 3.9751833386 -0.346514524 -0.6916895209

O 0.3161995123 2.386830317 -0.72387415
O 0.0059658986 -2.1844787973 0.6142134129
C -1.5036286765 0.3323963465 0.1503954889
S -2.7335380898 -0.9488410075 0.27711333
C -2.3377231042 -2.1106446604 -1.0820063756
N -2.0017803864 1.5634417724 0.2540005406
C -3.4058222538 1.9616897017 0.3107264342
H 3.4313256922 -0.4135444277 2.0489240084
H 1.9713775652 0.5987679262 2.0084846196
H 3.5408235038 1.2885588104 1.5375878016
H 4.5056217928 -1.1642745925 -0.1959285532
H 4.6197413652 0.5368400232 -0.7081380226
H 3.7423615482 -0.640518614 -1.7188435714
H -3.276450468 -2.6366625251 -1.2758456098
H -1.5563263745 -2.8042624164 -0.779852232
H -2.0464821528 -1.5554332996 -1.975754078
H -1.3043194385 2.3055225014 0.1722459987
H -3.8550641976 1.7102406418 1.2770181648
H -3.981114022 1.4753573482 -0.4818691374
H -3.442300684 3.0448075265 0.178631375

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B3LYP/6-31G(d) energy (a.u.): -1296.3794567

C 1.6617718324 0.2873248319 0.2667791554
C 0.889494666 -0.952214924 0.1647419546
O 3.0083223411 0.2123526582 0.0962665773
C 3.6791340606 -1.0284114509 0.3630687459
O 2.9666105498 -2.1243676581 -0.1961408239
C 1.6010872106 -2.2183221115 -0.0255389677
C 3.8263227828 -1.2113457518 1.8742796809
C 5.009946527 -0.9563274014 -0.3659756322
O 1.1973345855 1.4119026 0.4518149285
O 1.1205388538 -3.3321819741 -0.0707394232
C -0.5246028145 -0.8972300653 0.3079698546
S -1.6658857263 -2.1758916991 -0.1647225735
C -1.0428751425 -2.7897862049 -1.7736698949
N -1.0869202058 0.2185423957 0.8154828077
C -2.4476014028 0.5679192677 1.0135712598
C -3.3435430964 -0.2630036251 1.696243154
C -4.6557940692 0.160371312 1.9067541283
C -5.074275536 1.4162738702 1.4655929827
C -4.1698845546 2.2555289938 0.8104275178
C -2.861197152 1.836381485 0.5836477725
H 4.3569859755 -2.1444531484 2.0834443811
H 2.8452760183 -1.2558551459 2.3576657561
H 4.3871249636 -0.3746096282 2.3005097262
H 5.5700086524 -1.8819315421 -0.2082993469
H 5.5961101862 -0.1121318483 0.0070748822
H 4.8337674582 -0.8240592423 -1.4364777534
H -1.9398871188 -3.105319732 -2.313287171
H -0.3514280451 -3.6165075126 -1.6299285762
H -0.5618174977 -1.9787566455 -2.3236324076
H -0.3968306905 0.9778200724 0.9194035605
H -3.0112078298 -1.2199384151 2.0839586686
H -5.3471198805 -0.4917655384 2.4329141101
H -6.0954366211 1.7433587321 1.6389707253
H -4.4836797895 3.2381875006 0.4697757913
H -2.1554254906 2.4794555449 0.0650714493

11-SCRF

B3LYP/6-31G(d) energy (a.u.): -1296.3966742

C -1.4608027287 -1.2493952722 -0.4774531372
C -1.028987938 0.0917737501 -0.1010343622
O -2.7978259571 -1.4865915027 -0.5700282919
C -3.7080684495 -0.6745562632 0.1913967662
O -3.3515667509 0.7037293137 0.0884651653
C -2.0378094383 1.0919353729 0.2254219745
C -3.6863038607 -1.1161275792 1.6535597871
C -5.0685183069 -0.8248230643 -0.4651892382
O -0.722254099 -2.1896213202 -0.7737426726
O -1.8547376354 2.242444753 0.5878190217
C 0.3686905946 0.3711791788 -0.0196044849
S 1.0958932128 1.994362342 -0.0712870987
C 0.1480475092 2.8694910887 -1.3726093081
N 1.2433881173 -0.6411637293 0.0687077882
C 2.6687230975 -0.6114230604 0.1337524164
C 3.3351917749 0.0852443987 1.1476364687
C 4.7294883309 0.0474624345 1.2051884005
C 5.4538064734 -0.6987354664 0.2724932102
C 4.7800038152 -1.4129074949 -0.7229674516
C 3.3878315659 -1.3725978952 -0.7957263168
H -4.3944535699 -0.5145242526 2.2308389191
H -2.6883482264 -0.9907315411 2.08614091
H -3.9705979893 -2.1697263166 1.7291874742
H -5.805674017 -0.2165153687 0.0662159827
H -5.3835243183 -1.8716362568 -0.4353421031
H -5.0146797893 -0.495108485 -1.5063656598
H 0.8410786328 3.6251686201 -1.7525782515
H -0.7455973393 3.3309042183 -0.9589060648
H -0.1079912984 2.1797561231 -2.1792523615
H 0.8078485224 -1.5651429971 -0.0317135692
H 2.768250451 0.6288297517 1.9007956269
H 5.247342977 0.5925492929 1.9924800507
H 6.5407154022 -0.7309865444 0.3256043108
H 5.3385704497 -2.0008139926 -1.4492862397
H 2.8567327857 -1.9181582357 -1.5742456616

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B3LYP/6-31G(d) energy (a.u.): -1453.6419014

C 1.7314551696 0.1430529793 -0.5883264794
C 1.0588513933 -1.0908454844 -0.1903669597
O 3.0445598345 0.0521170237 -0.9309676787
C 3.7649643859 -1.1506216576 -0.6172988145
O 2.9918112069 -2.2984431208 -0.9606597045
C 1.6660119258 -2.3587256023 -0.5935441239
C 4.1395830084 -1.1670238663 0.8656488038
C 4.9761958327 -1.1626176884 -1.5349890449
O 1.2183169486 1.2589636373 -0.6658462256
O 1.1076850024 -3.4318937053 -0.7055665244
C -0.2609743358 -1.016601255 0.326486584
S -1.1306791216 -2.2941814717 1.1916925208
C 0.1429234694 -3.338287817 1.9795451306
N -0.9685177784 0.1175890464 0.1988106844
C -2.2110616648 0.4608176629 0.8396725655
C -2.1616119428 1.1142552168 2.0863078609
C -3.3756484756 1.4903031581 2.6697864451
C -4.5847654799 1.2322075062 2.0268470479

C -4.6057618194 0.6017376984 0.7848962295
C -3.4170400786 0.2074165693 0.1599618762
C -3.3973949527 -0.462897806 -1.2054545439
C -4.7532352881 -0.6092424408 -1.9014063006
C -0.8187244048 1.3770465232 2.7470637767
C -0.8512570343 2.2255239791 4.0209681119
H 4.6986098921 -2.079010394 1.0943716781
H 3.2469758619 -1.1356701368 1.496246549
H 4.7627003464 -0.2992752024 1.1005623417
H 5.5625262609 -2.0696752358 -1.364736728
H 5.6018745282 -0.2869230412 -1.3419394453
H 4.6446961347 -1.1430525255 -2.5760557996
H -0.3687846555 -3.8056073873 2.8250800003
H 0.9606655723 -2.7194246434 2.3555353351
H 0.5197314863 -4.0850365616 1.2835921426
H -0.4407544904 0.8578726389 -0.2877557578
H -3.379094726 1.9924415642 3.631381916
H -5.518780514 1.5324241707 2.4946174006
H -5.5565897996 0.4204347955 0.2957187212
H -2.9417449923 -1.4572797706 -1.1077954437
H -2.7184615936 0.0987692395 -1.8607667729
H -5.2338006249 0.3618478768 -2.0663657784
H -5.4431504615 -1.2349191099 -1.3239952376
H -4.6188522778 -1.0835786947 -2.8789916176
H -0.1514091948 1.8508299167 2.0154763307
H -0.349468071 0.4092201121 2.9756482614
H -1.4247652019 1.7425981599 4.8201465099
H -1.2908294943 3.2125806935 3.8383500227
H 0.167094214 2.3790604502 4.3929691344

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B3LYP/6-31G(d) energy (a.u.): -1453.6577978

C 1.7494394598 0.147621903 -0.5959216906
C 1.0572510337 -1.0736867949 -0.2109067788
O 3.0620874412 0.0411418958 -0.9355786236
C 3.769920524 -1.1738395798 -0.6238810075
O 2.9688727355 -2.304000278 -0.9885084433
C 1.6447879697 -2.3396000026 -0.6284147167
C 4.1301559475 -1.2131791204 0.859476966
C 4.9849479106 -1.1987726589 -1.533938276
O 1.2550269765 1.2741482777 -0.6711286251
O 1.0691237969 -3.4075358021 -0.7649597399
C -0.2612563607 -0.9878356785 0.3185002264
S -1.1034867482 -2.2655637399 1.2119214853
C 0.2029291626 -3.2508847083 2.0245742928
N -0.9740571337 0.1370597638 0.1881547706
C -2.2206479005 0.4644219936 0.8365686741
C -2.1712503254 1.1038612611 2.0906504342
C -3.3886734129 1.4583819727 2.682654934
C -4.5975833117 1.1942468257 2.0393933062
C -4.6162551399 0.5774776149 0.7892744412
C -3.4246410682 0.2028294719 0.1560274965
C -3.4012152693 -0.4550120807 -1.2157734711
C -4.755240341 -0.5923413648 -1.9172236536
C -0.8292753191 1.3751742575 2.7503829935
C -0.8668831692 2.2169942862 4.0285107233
H 4.673614804 -2.136389153 1.0809294612
H 3.2363928122 -1.1728009243 1.4876506611
H 4.7688709728 -0.360012475 1.1059322799

H 5.5556175167 -2.1162738703 -1.3651984856
H 5.6257005619 -0.3378277809 -1.3239730733
H 4.6648814993 -1.1625617305 -2.578775288
H -0.3050353871 -3.7408817587 2.8595558923
H 0.9832738809 -2.5959699664 2.4179557608
H 0.6221379296 -3.9871194489 1.3416996696
H -0.4870737914 0.8798683977 -0.3298003445
H -3.3993130751 1.9491688333 3.6511441314
H -5.5351775842 1.4790722893 2.514517963
H -5.5697324864 0.3926904264 0.3042593823
H -2.94869181 -1.452387524 -1.1261916839
H -2.7193904289 0.1123315243 -1.8639698103
H -5.2336318673 0.3816122514 -2.0711838949
H -5.4479727453 -1.2232145152 -1.34889738
H -4.6169771204 -1.0550306078 -2.9000457784
H -0.1686436312 1.8600368682 2.0195343356
H -0.349416478 0.4114118221 2.9744850383
H -1.4330609113 1.7236124155 4.8263796907
H -1.3181111049 3.1999944634 3.8519001644
H 0.1517349857 2.3778387486 4.3967905901

Rotational transition state for 7

B3LYP/6-31G(d) energy (a.u.): -1312.3792771
Imaginary frequency (cm^{-1}): -58.518

C 0.7201327316 -1.1265775543 -0.6367916246
C 0.8628787652 0.3187655536 -0.5144282187
O 1.7515329624 -1.8715791517 -0.1349696462
C 3.0224571178 -1.2475169204 0.0999940249
O 2.8648247178 0.0001444227 0.7859424356
C 1.8820525923 0.8658666871 0.3857238979
C 3.7561641425 -1.0301004335 -1.2242454266
C 3.7689809127 -2.1644009197 1.053902505
O -0.2598188177 -1.7124805576 -1.0704027407
O 1.927996452 2.0188453731 0.7662522118
C -0.2688228896 1.1467790901 -0.7189213496
S -1.0026106856 2.1204917727 0.6419448098
C -2.4624536577 1.0165279778 0.8822537303
N -0.8566168546 1.4170845293 -1.8905104237
C -0.5068182746 1.1129033406 -3.2335792413
C -0.8146901144 2.0915538878 -4.1897525073
C -0.4598793832 1.857843959 -5.51355576
N 0.1567040658 0.7443357065 -5.9342103015
C 0.419493596 -0.1834480874 -5.0095982291
C 0.108923338 -0.0661094653 -3.6508666288
H 4.7314124673 -0.573110381 -1.0343140066
H 3.1856040728 -0.3706486784 -1.8843151713
H 3.9040206713 -1.9894408729 -1.7288115537
H 4.7476693541 -1.7382575245 1.2903662357
H 3.9048539791 -3.1483235877 0.5966977859
H 3.1957021253 -2.275680863 1.97759918
H -2.9435602848 1.3693037499 1.7982669918
H -2.1391092101 -0.0172672565 1.0225536668
H -3.1775291009 1.0735567254 0.0575554786
H -1.6216067906 2.0813624398 -1.8143100218
H -1.2964260097 3.02344532 -3.905112274
H -0.6776530944 2.6050963361 -6.2739263019
H 0.8981569813 -1.092773453 -5.3677679368
H 0.2649491224 -0.8922901646 -2.9738585896

Rotational transition state for 8

B3LYP/6-31G(d) energy (a.u.): -1312.3807671

Imaginary frequency (cm⁻¹): -24.019

C 0.48207576 -0.3149038772 0.9631312855
C -0.2875357794 -1.5203477651 0.8354096224
O 1.8346209541 -0.4456120622 0.6716152075
C 2.4153477181 -1.7471077161 0.7588763646
O 1.6156181342 -2.7327235747 0.0894401039
C 0.2506323078 -2.727646663 0.3086210101
C 2.6183602436 -2.1450473697 2.2237963582
C 3.7232121918 -1.6774198015 -0.0156873573
O 0.0555055902 0.7973071457 1.2300336571
O -0.3717185309 -3.7459197815 -0.0067096681
C -1.7121614528 -1.4490021472 1.2036712484
S -1.9909877147 -1.6406960595 2.9170642577
C -3.7852195154 -1.3431746841 3.0979083665
N -2.7329697538 -1.1942917776 0.4368281431
C -2.7675057737 -1.1575756455 -0.9044264809
C -3.4839570633 -0.0989137432 -1.5402948343
C -3.5901788762 -0.0548513668 -2.9023170216
N -3.0305058682 -1.0357903845 -3.665921535
C -2.3539185705 -2.0776790013 -3.1013623522
C -2.2082713729 -2.168886128 -1.7449492884
H 3.0955983057 -3.1281560641 2.2800618454
H 1.6608056626 -2.190798849 2.7487432365
H 3.2550027142 -1.4083317481 2.7231574669
H 4.2189745097 -2.6523691104 -0.006023366
H 4.3853409354 -0.9316112927 0.4333083863
H 3.5176664221 -1.3922307894 -1.0508660738
H -3.9894857661 -1.3027269052 4.1709353688
H -4.3629165438 -2.1493215021 2.6411048305
H -4.0491520036 -0.3924235266 2.6293795544
H -3.9237961913 0.6821796512 -0.9319462371
H -4.1038488971 0.7359813326 -3.4356562246
H -3.1111491403 -0.9854110446 -4.6732860446
H -1.9393217717 -2.8057267544 -3.7890813145
H -1.6600968637 -2.996046994 -1.2918415152

Rotational transition state for 9

B3LYP/6-31G(d) energy (a.u.): -1311.8732019

Imaginary frequency (cm⁻¹): -60.812

C 1.0614400066 -0.8895003807 0.3514897706
C 0.3285046904 -0.2705881091 1.4486390503
O 2.1050168803 -1.7477639496 0.7253934561
C 2.620537917 -1.6556630864 2.0433842838
O 1.5723829791 -1.6343996689 3.007068311
C 0.5148129854 -0.7542857526 2.7977698276
C 3.506197984 -0.4108612053 2.1908454316
C 3.391518314 -2.9467229339 2.2902284654
O 0.8571600297 -0.7925750276 -0.8400963205
O -0.1723354993 -0.5029724129 3.7756863437
C -0.6190738373 0.762103689 1.1500661165
S -1.6398452894 1.3960967032 2.550123211
C -2.5297976165 2.7175211808 1.6512049642
N -0.7367973673 1.3805736481 0.024524773
C -1.3845503685 1.3119571024 -1.1389884444
C -1.2000118316 2.3004252473 -2.1456019658
C -1.921349225 2.2264989421 -3.3251343113

N -2.8232132771 1.2743669834 -3.6322602096
C -2.9875949282 0.3350736542 -2.6814989399
C -2.3266654357 0.2936742917 -1.4646437168
H 3.9215814576 -0.3634957289 3.2028397729
H 2.9230902847 0.4956247034 2.0088732631
H 4.3265818404 -0.4494883701 1.4668927965
H 3.8042856604 -2.9525215153 3.3038420936
H 4.2072045656 -3.0421139105 1.5669486677
H 2.7140874682 -3.7972097223 2.1762701987
H -3.1143658837 3.2473352403 2.4108789017
H -3.2029362783 2.3166940352 0.8900651956
H -1.8295344989 3.4068868088 1.173657102
H -0.4899030236 3.1049803955 -1.9754615821
H -1.7692406336 2.9935283061 -4.0879021583
H -3.7087487241 -0.4508389674 -2.9168602392
H -2.5095873452 -0.5114811898 -0.7592571087

4-Aminopyridine

B3LYP/6-31G(d) energy (a.u.): -303.6427991

N 0.4322633754 1.8114723889 0.0231879039
C 0.2207162129 0.4429337264 0.010587136
C 0.9227541721 -0.4170006596 0.8729802527
C 0.707174433 -1.7875045903 0.7792897569
N -0.1358204532 -2.3697772739 -0.0853397251
C -0.7986544215 -1.5392612409 -0.9027497009
C -0.6659881959 -0.155088571 -0.9016547276
H 0.8155416689 2.1987608985 0.875316336
H -0.3020704041 2.3830179285 -0.3731797318
H 1.6266444773 -0.0190901679 1.5999757914
H 1.2462839746 -2.4603768226 1.4452687878
H -1.4850527622 -2.0101038881 -1.6056638614
H -1.2372150774 0.453029272 -1.5989422179

4-Aminopyridine SCRF

B3LYP/6-31G(d) energy (a.u.): -303.6592717

N 0.4248399942 1.804756783 0.0287175299
C 0.2166911191 0.4466886154 0.0148415546
C 0.9209330893 -0.4191037543 0.8774059277
C 0.7111295632 -1.7882183856 0.7800695165
N -0.1312821432 -2.3759666875 -0.0903357273
C -0.7990202918 -1.5392124471 -0.9068484752
C -0.6706857354 -0.1566868887 -0.9006240461
H 0.8317993322 2.2026871371 0.8725663123
H -0.297493061 2.3885413505 -0.3879599853
H 1.6202042317 -0.0191075511 1.6103988484
H 1.2540955737 -2.4595995809 1.4479448846
H -1.4867408385 -2.0076294112 -1.6134246665
H -1.2478938336 0.4538618204 -1.5936756735

4-Aminopyridinium cation

B3LYP/6-31G(d) energy (a.u.): -304.0370716

N 0.4297783836 2.31123875 0.022908679
C 0.2128575626 0.9903306661 0.0223563264
C 0.9280450868 0.1235865775 0.8983773775
C 0.6847345415 -1.2222503112 0.8749544107
N -0.2361223596 -1.7441292198 0.0211448172
C -0.9416320482 -0.9544556282 -0.8320815711

C -0.7418171388 0.3985432091 -0.8543044135
H 1.1057549253 2.7372995353 0.6427290822
H -0.07460475 2.9316571059 -0.5962268138
H 1.6668309931 0.5177752244 1.5874661732
H 1.2006354417 -1.9237101109 1.519620014
H -1.6546575462 -1.4535622815 -1.4772797118
H -1.315669234 1.0088686244 -1.5429473286
H -0.4004518577 -2.7451191414 0.0206769586

4-Aminopyridinium cation SCRF

B3LYP/6-31G(d) energy (a.u.): -304.1322749

N 0.4298922143 2.312062102 0.0229277661
C 0.2131428832 0.9920566404 0.0223614146
C 0.9281566078 0.1253778442 0.8982118138
C 0.6829052244 -1.2210765711 0.8733035391
N -0.2359115523 -1.7428561122 0.0211404012
C -0.9395235381 -0.9539362932 -0.8304424815
C -0.7413354847 0.4002675151 -0.8541376954
H 1.1131405114 2.7359253079 0.6485700837
H -0.0820385504 2.9327146369 -0.6020794614
H 1.6683857493 0.5261835243 1.5875986615
H 1.1979291043 -1.9289740368 1.5183181812
H -1.6537786258 -1.4594181532 -1.4759963877
H -1.3144403534 1.0173289482 -1.5430680602
H -0.40284219 -2.7595823527 0.020686225