A Facile One-Pot Coupling-Aminovinylation Approach to Push-Pull Chromophores – Alkyne Activation by Sonogashira-Coupling

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SUPPORTING INFORMATION

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I. Computational Data

Computer programs: a) PC Spartan Pro, Wavefunction, Inc., **1999**, Irvine, CA, U.S.A..

b) Quantum CAChe 3.0, Oxford Molecular, **1997**.

Methods applied: a) equilibrium geometries by semi-empirical PM3 and AM1 methods (implemented in PC Spartan Pro)

b) transition state geometries by the semi-empirical PM3 method (implemented in PC Spartan Pro)

c) UV/vis transitions by ZINDO/CI calculations (implemented in Quantum CAChe 3.0)

1. Equilibrium geometries of the structures **3** (PM3)

Compound **3a**:

Cartesian Coordinates (Angstroms)

Atom Label	X	Y	Z
-----	-----	-----	-----
H H1	1.5742271	0.0000000	4.9747959
C C1	0.7061620	0.0000000	4.3205561
C C2	-1.5224724	0.0000000	2.6398478
C C3	0.8771080	0.0000000	2.9344058
C C4	-0.5777052	0.0000000	4.8657634
C C5	-1.6916644	0.0000000	4.0262308
C C6	-0.2374271	0.0000000	2.0920550
H H2	1.8819737	0.0000000	2.5195205
H H3	-0.7101124	0.0000000	5.9452632
H H4	-2.6924007	0.0000000	4.4507180
C C7	-0.0634520	0.0000000	0.6721181
H H6	-2.3971541	0.0000000	1.9937758
C C8	0.0820294	0.0000000	-0.5203507
C C9	0.2581847	0.0000000	-1.9350573
C C10	1.4793854	0.0000000	-2.5774511
C C11	1.3401455	0.0000000	-3.9994489
C C12	0.0130979	0.0000000	-4.3734249
S S1	-1.0447455	0.0000000	-3.0436386
H H10	2.4303177	0.0000000	-2.0563931
H H13	2.1690365	0.0000000	-4.6987961
N N1	-0.4977620	0.0000000	-5.7196574
O O1	0.3473211	0.0000000	-6.6256516
O O2	-1.7240932	0.0000000	-5.8851810

Total energy: 102.554 kcal/mol

Compound **3b**:

Cartesian Coordinates (Angstroms)

Atom Label	X	Y	Z
-----	-----	-----	-----
H H1	-2.1835424	-0.6908834	-4.6764366
C C1	-1.3286380	-0.2586547	-4.1454297
C C2	0.8518895	0.8465472	-2.8019619
C C3	-1.2402422	-0.3803053	-2.7638438
C C4	-0.3356546	0.4097888	-4.8549200

C	C5	0.7511487	0.9611960	-4.1832313
C	C6	-0.1464532	0.1732132	-2.0889610
H	H2	-2.0213122	-0.9059627	-2.2045796
H	H3	-0.4099519	0.5024203	-5.9434534
H	H4	1.5307024	1.4875541	-4.7438770
C	C7	-0.0494339	0.0517966	-0.6827768
H	H6	1.7070463	1.2803070	-2.2723472
C	C8	0.0371766	-0.0486439	0.5061498
C	C9	0.1221551	-0.1720674	1.8975999
C	C10	-0.8008265	-0.8155361	2.6927683
C	C11	-0.4460409	-0.7748210	4.0750327
C	C12	0.7336209	-0.1043691	4.2982310
S	S1	1.4356996	0.4892613	2.8274447
H	H10	-1.7036475	-1.3036097	2.3228370
H	H13	-1.0527055	-1.2289591	4.8621851
C	C13	1.3601966	0.1089774	5.6136256
O	O1	0.8791301	-0.2959569	6.6475780
H	H8	2.3096830	0.6687073	5.6183662

Total energy: 74.628 kcal/mol

Compound 3c:

Cartesian Coordinates (Angstroms)

Atom Label	X	Y	Z

H H1	-3.7592584	1.6855025	-2.8138494
C C1	-3.3476472	0.8381240	-2.2555000
C C2	-2.3076737	-1.3262188	-0.8358437
C C3	-2.1297923	0.9696090	-1.5992228
C C4	-4.0445142	-0.3653606	-2.2052946
C C5	-3.5244829	-1.4441740	-1.4966328
C C6	-1.6072232	-0.1157587	-0.8868141
H H2	-1.5806455	1.9164388	-1.6381588
H H3	-5.0036955	-0.4636254	-2.7243268
H H4	-4.0750375	-2.3900126	-1.4587383
C C7	-0.3678602	0.0110856	-0.2167243
H H6	-1.8976895	-2.1746989	-0.2778676
C C8	0.6807259	0.1231478	0.3482083
C C9	1.9057638	0.2373562	1.0143962
C C10	2.5055834	-0.7649995	1.7448249
C C11	3.7506944	-0.3566316	2.3100855
C C12	4.0629031	0.9462857	1.9931847
S S1	2.8499180	1.7004989	1.0022352
H H10	2.0884276	-1.7633011	1.8846206
H H13	4.3705948	-1.0152818	2.9208530
C C13	5.2320624	1.6087694	2.4173741
N N1	6.1988464	2.1432449	2.7731908

Total energy: 145.106 kcal/mol

Compound **3d**:

Cartesian Coordinates (Angstroms)

Atom Label		X	Y	Z
-----		-----	-----	-----
H	H1	-0.1666772	2.4829284	-4.3574060
C	C1	-0.2355919	1.4831307	-3.9160563
C	C2	-0.4125453	-1.0680466	-2.8018296
C	C3	-0.1116621	1.3251745	-2.5411334
C	C4	-0.4467210	0.3761508	-4.7324474
C	C5	-0.5347191	-0.8958553	-4.1752225
C	C6	-0.2004377	0.0456254	-1.9813734
H	H2	0.0546120	2.1955022	-1.8973697
H	H3	-0.5438119	0.5063163	-5.8153560
H	H4	-0.7007682	-1.7650901	-4.8201422
C	C7	-0.0752714	-0.1217849	-0.5819210
H	H6	-0.4815306	-2.0687205	-2.3622306
C	C8	0.0305637	-0.2613783	0.6003493
C	C9	0.1518458	-0.4461482	1.9860337
C	C10	0.0921176	-1.5834317	2.7691265
C	C11	0.2865558	-1.1497138	4.1218003
C	C12	0.4519383	0.2191992	4.0783317
O	O2	0.3724939	0.6749727	2.7693200
H	H10	-0.0690908	-2.6061761	2.4394327
H	H13	0.2997234	-1.7841226	5.0054074
C	C13	0.6860332	1.2297696	5.1231909
O	O1	0.7711893	0.9342688	6.2936048
H	H8	0.7817533	2.2774296	4.7958907

Total energy: 39.900 kcal/mol

Compound **3e**:

Cartesian Coordinates (Angstroms)

Atom Label		X	Y	Z
-----		-----	-----	-----
H	H1	-2.2448696	0.0000000	-4.5290268
C	C1	-1.2938506	0.0000000	-3.9863680
C	C2	1.1334313	0.0000000	-2.6132741
C	C3	-1.2917047	0.0000000	-2.5967771
C	C4	-0.0929679	0.0000000	-4.6891176
C	C5	1.1172834	0.0000000	-4.0026958
C	C6	-0.0743142	0.0000000	-1.9067207
H	H2	-2.2358448	0.0000000	-2.0413726
H	H3	-0.1003045	0.0000000	-5.7839413
H	H4	2.0607995	0.0000000	-4.5581687
C	C7	-0.0675382	0.0000000	-0.4914370
H	H6	2.0854032	0.0000000	-2.0722291
C	C8	-0.0629364	0.0000000	0.7033177
C	C9	-0.0615770	0.0000000	2.1211313
C	C10	-0.1402316	0.0000000	4.8733584
N	N1	-1.2698725	0.0000000	2.7555486
C	C12	1.1417041	0.0000000	2.8404261
C	C13	1.0929802	0.0000000	4.2314134
C	C14	-1.3064769	0.0000000	4.1037228
H	H10	2.1009148	0.0000000	2.3129933
H	H11	2.0201512	0.0000000	4.8137338
H	H12	-2.3078032	0.0000000	4.5496306

H	H13	-0.2023757	0.0000000	5.9658529
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Total energy: 106.126 kcal/mol

Compound 3f:

Cartesian Coordinates (Angstroms)

Atom Label	X	Y	Z
H H1	2.0383840	0.0000000	-1.5796953
C C1	1.0661059	0.0000000	-2.0844177
C C2	-1.4138587	0.0000000	-3.3620456
C C3	-0.1137572	0.0000000	-1.3319000
C C4	0.9951132	0.0000000	-3.4724201
C C5	-0.2411216	0.0000000	-4.1110462
C C6	-1.3573504	0.0000000	-1.9735073
H H3	1.9164288	0.0000000	-4.0642946
H H4	-0.2913074	0.0000000	-5.2048550
H H5	-2.2797983	0.0000000	-1.3831704
H H6	-2.3853593	0.0000000	-3.8672541
C C9	0.0883352	0.0000000	2.6773285
N N3	1.2509241	0.0000000	3.3365845
C C11	1.0545796	0.0000000	4.7249291
C C12	-0.2631576	0.0000000	5.0969303
S S1	-1.3260055	0.0000000	3.7386597
H H13	1.9288393	0.0000000	5.3796130
C C8	-0.0465481	0.0000000	0.0814348
C C7	0.0072033	0.0000000	1.2760073
H H2	-0.6276493	0.0000000	6.1231190

Total energy: 117.645 kcal/mol

Compound 3g:

Cartesian Coordinates (Angstroms)

Atom Label	X	Y	Z
H H1	2.1532472	0.0000000	5.1954353
C C1	1.2057914	0.0000000	4.6462614
C C2	-1.2128288	0.0000000	3.2565374
C C3	1.2128288	0.0000000	3.2565374
C C4	0.0000000	0.0000000	5.3408313
C C5	-1.2057914	0.0000000	4.6462614
C C6	0.0000000	0.0000000	2.5585237
H H2	2.1613610	0.0000000	2.7090859
H H3	0.0000000	0.0000000	6.4358913
H H4	-2.1532472	0.0000000	5.1954353
C C7	0.0000000	0.0000000	1.1433107
H H6	-2.1613610	0.0000000	2.7090859
C C8	0.0000000	0.0000000	-0.0521867
C C9	0.0000000	0.0000000	-1.4660836
C C10	0.0000000	0.0000000	-4.2565252
C C11	1.2118415	0.0000000	-2.1667187
C C12	-1.2118415	0.0000000	-2.1667187
C C13	-1.2119004	0.0000000	-3.5543363
C C14	1.2119004	0.0000000	-3.5543363

H	H9	2.1611881	0.0000000	-1.6191986
H	H10	-2.1611881	0.0000000	-1.6191986
H	H11	-2.1707956	0.0000000	-4.0920423
H	H12	2.1707956	0.0000000	-4.0920423
N	N1	0.0000000	0.0000000	-5.7524986
O	O1	1.0581548	0.0000000	-6.3506554
O	O2	-1.0581548	0.0000000	-6.3506554

Total energy: 89.517 kcal/mol

Compound 3h:

Cartesian Coordinates (Angstroms)

Atom	Label	X	Y	Z
H	H1	2.0028669	0.0000000	-2.3267931
C	C1	1.0097580	0.0000000	-2.7895411
C	C2	-1.5233712	0.0000000	-3.9608586
C	C3	-0.1379685	0.0000000	-1.9883858
C	C4	0.8797355	0.0000000	-4.1732290
C	C5	-0.3828753	0.0000000	-4.7585725
C	C6	-1.4083575	0.0000000	-2.5760341
H	H3	1.7751969	0.0000000	-4.8038783
H	H4	-0.4793813	0.0000000	-5.8495346
H	H5	-2.3053598	0.0000000	-1.9474484
H	H6	-2.5154910	0.0000000	-4.4247446
C	C9	0.2388379	0.0000000	2.0060750
N	N3	1.4472415	0.0000000	2.6014467
C	C11	1.3357155	0.0000000	3.9825255
C	C12	0.0248161	0.0000000	4.4419543
S	S1	-1.1114651	0.0000000	3.1179876
H	H13	2.2468926	0.0000000	4.5936560
N	N1	-0.3089988	0.0000000	5.8905004
O	O1	0.6016107	0.0000000	6.6935940
O	O2	-1.4704257	0.0000000	6.2385352
C	C8	-0.0108275	0.0000000	-0.5798762
C	C7	0.0918499	0.0000000	0.6126216

Total energy: 113.889 kcal/mol

Compound 3i:

Cartesian Coordinates (Angstroms)

Atom	Label	X	Y	Z
H	H1	-2.3039827	0.0000000	5.0621984
C	C1	-1.3435398	0.0000000	4.5359401
C	C2	1.1081102	0.0000000	3.2049069
C	C3	-1.3175466	0.0000000	3.1463584
C	C4	-0.1547150	0.0000000	5.2591494
C	C5	1.0676432	0.0000000	4.5939853
C	C6	-0.0878193	0.0000000	2.4782741
H	H2	-2.2523515	0.0000000	2.5750323
H	H3	-0.1809814	0.0000000	6.3539367
H	H4	2.0015215	0.0000000	5.1659366
C	C7	-0.0566558	0.0000000	1.0635449

H	H6	2.0696317	0.0000000	2.6807101
C	C8	-0.0309765	0.0000000	-0.1316660
C	C9	-0.0101868	0.0000000	-1.5465923
C	C10	-0.0569620	0.0000000	-4.3055203
N	N2	-1.2101237	0.0000000	-2.1998941
C	C12	1.2019338	0.0000000	-2.2536704
C	C13	1.1766805	0.0000000	-3.6420342
C	C14	-1.2404087	0.0000000	-3.5441505
H	H10	2.1556214	0.0000000	-1.7143181
H	H11	2.1205875	0.0000000	-4.2057168
H	H12	-2.2444715	0.0000000	-3.9947659
N	N1	-0.1205289	0.0000000	-5.7982392
O	O1	-1.2038739	0.0000000	-6.3469260
O	O2	0.9133944	0.0000000	-6.4364794

Total energy: 98.134 kcal/mol

2. Transition state geometries and energies of the aminovinylolation of **3a** with pyrrolidine in the presence of one molecule of methanol (PM3)

a) **3a** + pyrrolidine + MeOH (educts):

Cartesian Coordinates (Angstroms)

Atom Label	X	Y	Z

H H1	-1.2540804	1.6935475	1.5296939
C C1	-0.6905231	2.2557270	2.2916147
C C2	0.7348125	3.6786011	4.2221127
C C3	0.7068238	2.1918708	2.3241835
C C4	-1.3644254	3.0322950	3.2263846
C C5	-0.6549947	3.7428556	4.1899274
C C6	1.4213293	2.9058272	3.2932866
H H3	-2.4581441	3.0843128	3.2024073
H H4	-1.1911202	4.3538240	4.9238031
H H5	2.5153788	2.8552896	3.3177576
H H6	1.2910906	4.2389563	4.9813012
C C9	2.7096312	-0.0081012	-0.3663998
C C10	2.1284530	-0.7054446	-1.4070419
C C11	3.0901238	-1.3798904	-2.2050959
C C12	4.3862240	-1.1854267	-1.7578300
S S1	4.4321459	-0.1666977	-0.3455850
H H10	1.0524383	-0.7450496	-1.6089082
H H13	2.8146258	-1.9830930	-3.0776318
N N1	5.5609112	-1.7924259	-2.4353665
O O1	5.3746266	-2.4697405	-3.4271747
O O2	6.6757666	-1.6056821	-1.9946235
H H2	-0.5570290	-0.3443356	0.1636557
C C13	-1.4852289	-0.8198327	-0.2145153
C C15	-3.2431229	-2.1977140	0.6602294
C C16	-3.8220145	-0.7878773	0.5240562
C C17	-2.7091547	0.0832644	-0.0558881
H H7	-1.2963180	-1.0662783	-1.2838379
H H11	-3.6218606	-2.8693685	-0.1337521
H H12	-3.5055016	-2.6736524	1.6232766
H H14	-4.1641611	-0.3981506	1.5009978
H H15	-4.7184016	-0.7854391	-0.1222990
H H16	-2.4835791	0.9444428	0.6095700
H H17	-3.0033904	0.5302382	-1.0227618
H H8	-1.1037818	-2.6323290	-4.2703201
C C14	-0.5158457	-1.7986940	-3.8684604

H	H18	0.5334362	-2.1101006	-3.7708164
H	H20	-0.9033604	-1.5208812	-2.8773889
O	O3	-0.6447781	-0.6373494	-4.6302926
N	N3	-1.7681919	-2.1029719	0.4843793
C	C7	1.4033591	1.4073416	1.3747654
C	C8	2.0080863	0.7525000	0.5760918
H	H27	-1.3121652	-2.1209572	1.3706193
H	H29	-0.3680712	-0.8434095	-5.5141244

Total energy: 31.785 kcal/mol

b) **5a** + MeOH (products):

Cartesian Coordinates (Angstroms)

Atom Label	X	Y	Z

H H1	-2.4111148	2.0883066	0.2060868
C C1	-2.4410737	1.3152130	0.9821550
C C2	-2.5205622	-0.6563327	2.9503670
C C3	-1.5847598	0.2142991	0.9056097
C C4	-3.3319874	1.4239755	2.0444589
C C5	-3.3728161	0.4403901	3.0273538
C C6	-1.6259662	-0.7734572	1.8921202
H H3	-4.0032013	2.2870420	2.1051312
H H4	-4.0757257	0.5296947	3.8622804
H H5	-0.9507405	-1.6344469	1.8343752
H H6	-2.5514046	-1.4298723	3.7250125
C C18	0.6785539	0.4094201	-0.1230011
C C9	1.3278862	0.9823613	1.0240759
C C10	0.7880362	1.8243412	1.9747830
C C11	1.7312379	2.2288821	2.9545695
C C12	2.9901582	1.6935463	2.7404229
S S1	3.0122147	0.6788537	1.3227216
H H10	-0.2564621	2.1495231	1.9799868
H H13	1.4753196	2.8967329	3.7833082
N N1	4.1408279	1.9763552	3.6272261
O O1	3.9786187	2.7141390	4.5804978
O O2	5.2227348	1.4745873	3.3978280
H H2	-0.4431337	0.2823756	-3.3196627
C C13	-0.3605224	-0.5896579	-2.6427167
C C15	-2.3356340	-1.3129642	-1.4264866
C C16	-1.9649025	-2.4283881	-2.3989429
C C17	-0.8677166	-1.8710495	-3.2997947
H H7	0.7215418	-0.6615378	-2.3692248
H H11	-2.5227212	-1.6947817	-0.4025567
H H12	-3.2581994	-0.7861635	-1.7392196
H H14	-2.8434325	-2.7610158	-2.9810591
H H15	-1.6141342	-3.3267117	-1.8560462
H H16	-1.2534788	-1.6637746	-4.3157080
H H17	-0.0490889	-2.6008776	-3.4406074
H H8	3.9921772	-1.2323939	-2.0909631
C C14	3.4375852	-0.4743361	-2.6569806
H H18	3.9662039	0.4843338	-2.5937912
H H20	2.4281354	-0.3623055	-2.2239335
O O3	3.2067950	-0.8662812	-3.9761835
H H19	4.0522562	-0.9658338	-4.3950436
H H22	1.3533477	0.2186107	-0.9847438
C C19	-0.6371244	0.0893681	-0.2235792
N N2	-1.2277064	-0.3101696	-1.4601254

Total energy: 4.511 kcal/mol

c) zwitter ion + MeOH (intermediate): Total energy: 49.077 kcal/mol

Cartesian Coordinates (Angstroms)

Atom Label		X	Y	Z
--		-----	-----	-----
H	H1	2.0279048	-0.3580937	-1.8305871
C	C1	1.1135409	0.0925425	-2.2332942
C	C2	-1.1870665	1.2978683	-3.2439333
C	C3	0.0469344	0.3862660	-1.3799189
C	C4	1.0228198	0.3999842	-3.5865512
C	C5	-0.1250194	1.0013624	-4.0924898
C	C6	-1.1031001	0.9927100	-1.8908343
H	H3	1.8629951	0.1760209	-4.2527097
H	H4	-0.1901601	1.2480726	-5.1574831
H	H5	-1.9385067	1.2276876	-1.2152446
H	H6	-2.0873671	1.7793938	-3.6399107
C	C9	1.6812992	1.6545112	1.5627977
C	C10	1.2450882	2.8072979	2.2467809
C	C11	2.2849771	3.4879822	2.8819468
C	C12	3.5353329	2.8852073	2.7230630
S	S1	3.4104972	1.4405104	1.7270281
H	H10	0.2072688	3.1362957	2.2581453
H	H13	2.1304703	4.4075107	3.4545657
N	N1	4.7541170	3.4116554	3.3116474
O	O1	4.7050618	4.4310639	3.9848056
O	O2	5.8227585	2.8451338	3.1490714
H	H2	-2.4513432	-0.6547630	1.5972070
C	C13	-2.0789519	-0.9150176	0.5842951
C	C15	-0.2424078	-2.3727467	-0.0990747
C	C16	-1.5165099	-3.2079342	-0.0843960
C	C17	-2.6721192	-2.2240600	0.0698677
H	H7	-2.3517809	-0.0520092	-0.0696228
H	H11	0.0882935	-2.1438714	-1.1367791
H	H12	0.6111323	-2.8889460	0.3842017
H	H14	-1.5018401	-3.9404853	0.7459086
H	H15	-1.6090795	-3.8097390	-1.0069559
H	H16	-3.4454272	-2.6128449	0.7577754
H	H17	-3.1897319	-2.0633617	-0.8950308
N	N2	-0.5642780	-1.0768101	0.6267558
H	H18	-0.2892418	-1.1659646	1.6146268
C	C7	0.1850639	0.1276376	0.0597337
C	C19	0.8798160	0.7685827	0.9380908
O	O3	0.0592428	-1.2408617	3.3926421
C	C8	-0.5088994	-0.1180189	4.0171134
H	H9	-0.1532267	0.8203498	3.5650894
H	H19	-0.3043986	-0.1141547	5.0935968
H	H20	-1.5852324	-0.2278768	3.8499379
H	H21	1.0012203	-1.1677963	3.5046538

Total energy: 49.077 kcal/mol

d) (**3a** + pyrrolidine + MeOH $\rightarrow$ **5a** + MeOH)[‡] (stationary point, concerted reaction (six-membered transition state):

Cartesian Coordinates (Angstroms)

Atom Label		X	Y	Z
-----		-----	-----	-----
H	H1	-1.8820462	-1.5749369	0.1042102
C	C1	-1.8082124	-1.0434951	1.0643253
C	C2	-1.5860584	0.2879313	3.4972895
C	C3	-0.7048823	-0.2228621	1.3097202
C	C4	-2.7951986	-1.1929004	2.0311829
C	C5	-2.6853870	-0.5268949	3.2476205
C	C6	-0.5958998	0.4425165	2.5329979
H	H3	-3.6615084	-1.8322571	1.8323573
H	H4	-3.4660407	-0.6414241	4.0068581
H	H5	0.2618113	1.0976261	2.7239360
H	H6	-1.5015312	0.8157021	4.4531862
C	C18	0.4880492	1.0361863	-0.5143340
C	C9	-0.2880870	2.2204448	-0.6048756
C	C10	-1.4582885	2.3560895	-1.3308560
C	C11	-1.9564860	3.6806168	-1.3222041
C	C12	-1.1641271	4.5504720	-0.5880570
S	S1	0.2189104	3.7239670	0.0925615
H	H10	-1.9529441	1.5350471	-1.8501809
H	H13	-2.8745965	3.9729095	-1.8409534
N	N1	-1.4854853	5.9788355	-0.4274153
O	O1	-2.4842075	6.4231775	-0.9651938
O	O2	-0.7633628	6.7004338	0.2329865
H	H2	-0.3790903	-2.3548409	-0.4391513
C	C13	0.7345225	-2.3813916	-0.4925417
C	C15	2.1014210	-1.4600615	1.3059516
C	C16	2.3782866	-2.9567205	1.2312165
C	C17	1.3137972	-3.5433639	0.3093777
H	H7	0.9865769	-2.4469882	-1.5697223
H	H11	3.0277583	-0.8554327	1.3476628
H	H12	1.5169367	-1.1945725	2.2131280
H	H14	2.3533118	-3.4198429	2.2343867
H	H15	3.3951604	-3.1533765	0.8403807
H	H16	0.5203383	-4.0492632	0.8918347
H	H17	1.7343482	-4.3217642	-0.3533018
H	H8	2.7047616	0.8525816	-3.6876860
C	C14	2.6045746	-0.0347989	-3.0550579
H	H18	3.4836054	-0.6750543	-3.1744047
H	H20	1.7027209	-0.5909275	-3.3397842
O	O3	2.5687108	0.3708873	-1.7129498
H	H19	2.1814847	-0.5787693	-0.8832895
H	H22	1.7176636	0.9617557	-1.4610886
C	C19	0.3199721	-0.0224270	0.2741737
N	N2	1.3309168	-1.1020181	0.0569599

Total energy: 63.240 kcal/mol
one imaginary vibration: i2364.13 cm⁻¹

e) (**3a** + pyrrolidine + MeOH $\rightarrow$ **5a** + MeOH)[‡]: (stationary point, concerted reaction (four-membered transition state):

Cartesian Coordinates (Angstroms)				
Atom Label		X	Y	Z

H	H1	1.0376598	-1.5239301	2.0269305
C	C1	1.5889502	-1.8034850	1.1174794
C	C2	3.0141399	-2.4826741	-1.1757164
C	C3	1.1364883	-1.3769375	-0.1335923
C	C4	2.7435057	-2.5710572	1.2159239
C	C5	3.4554305	-2.9136882	0.0711710
C	C6	1.8601794	-1.7153353	-1.2816383
H	H3	3.0958184	-2.9006669	2.1989531
H	H4	4.3657101	-3.5168363	0.1520277
H	H5	1.5207699	-1.3588366	-2.2619235
H	H6	3.5789956	-2.7437946	-2.0768095
C	C9	0.3583202	1.6346854	-1.5173749
C	C10	0.8363143	1.5724006	-2.8149249
C	C11	1.3965487	2.7976817	-3.2482642
C	C12	1.3484578	3.7873404	-2.2775234
S	S1	0.5872890	3.2029843	-0.8155743
H	H10	0.7925187	0.6788338	-3.4391017
H	H13	1.8261638	2.9342012	-4.2454985
N	N1	1.8860518	5.1422273	-2.4909883
O	O1	2.3963337	5.4133088	-3.5629090
O	O2	1.8176040	5.9742483	-1.6067582
H	H2	-0.6536553	-1.2380564	2.2009093
C	C13	-1.6167777	-0.9941852	1.6972309
C	C15	-1.9766596	-2.2158675	-0.3798056
C	C16	-2.6696021	-2.9778156	0.7477184
C	C17	-2.6774803	-2.0545810	1.9620902
H	H7	-1.9083207	0.0162604	2.0663470
H	H11	-2.6757146	-1.9567757	-1.1981543
H	H12	-1.1627033	-2.8097971	-0.8422070
H	H14	-2.1351628	-3.9212360	0.9690594
H	H15	-3.6933345	-3.2802801	0.4604381
H	H16	-2.4706768	-2.6041158	2.8984478
H	H17	-3.6731739	-1.5924167	2.1050606
H	H8	-2.2706886	3.4902601	2.3027240
C	C14	-1.5044027	2.7082570	2.2422928
H	H18	-0.8415479	2.9124271	1.3860112
H	H20	-1.9897275	1.7322736	2.0980117
O	O3	-0.8065402	2.5678387	3.4433303
N	N3	-1.4247886	-0.9375949	0.2011010
C	C7	-0.0519672	-0.5507739	-0.2760364
C	C8	-0.3309206	0.6192414	-0.8329462
H	H27	-1.7417953	0.1387838	-0.3335054
H	H29	-0.3082277	3.3644838	3.5752783

Total energy: 60.524 kcal/mol

One imaginary vibration: i1678.26 cm⁻¹

f) (**3a** + pyrrolidine + MeOH $\rightarrow$ zwitter ion + MeOH)[‡] (stationary point, amine addition):

Cartesian Coordinates (Angstroms)

Atom Label		X	Y	Z
-----		-----	-----	-----
H	H1	0.7759100	-1.7481438	1.6173652
C	C1	1.3307358	-2.1618705	0.7615200
C	C2	2.6972212	-3.2124146	-1.4265947
C	C3	1.2363896	-1.5379923	-0.4865049
C	C4	2.1103183	-3.3025142	0.9096057
C	C5	2.7943303	-3.8275419	-0.1824746
C	C6	1.9212624	-2.0696116	-1.5841328
H	H3	2.1881980	-3.7857079	1.8892278
H	H4	3.4115357	-4.7240492	-0.0619331
H	H5	1.8575871	-1.5761203	-2.5604006
H	H6	3.2382740	-3.6250318	-2.2847944
C	C9	0.8398643	2.2756246	-0.9036136
C	C10	0.8253879	3.1919550	0.1468257
C	C11	1.0533524	4.5135510	-0.2814178
C	C12	1.2334954	4.6211276	-1.6558134
S	S1	1.1347129	3.0543490	-2.4312013
H	H10	0.6547349	2.9132848	1.1920023
H	H13	1.0806641	5.3644548	0.4061010
N	N1	1.4737034	5.9031421	-2.3287207
O	O1	1.5164411	6.9232169	-1.6620566
O	O2	1.6236848	5.9479485	-3.5353743
H	H2	-0.9444622	-1.4210446	1.3415876
C	C13	-1.7824340	-0.9833323	0.7486361
C	C15	-1.6750786	-1.8696793	-1.4927217
C	C16	-2.8239916	-2.5849365	-0.7818194
C	C17	-2.9467349	-1.9587856	0.6068130
H	H7	-2.0583697	-0.0421844	1.2768741
H	H11	-1.9480487	-1.5366200	-2.5124281
H	H12	-0.7892597	-2.5288633	-1.6104013
H	H14	-2.6299496	-3.6716772	-0.7194135
H	H15	-3.7687770	-2.4884569	-1.3487163
H	H16	-2.9220005	-2.7235759	1.4044392
H	H17	-3.9175977	-1.4415511	0.7266399
H	H8	-1.6316232	2.5181660	3.6158714
C	C14	-1.0293521	1.7764756	3.0784593
H	H18	-0.2338390	2.2915785	2.5145815
H	H20	-1.6686462	1.2262288	2.3736101
O	O3	-0.5268297	0.7879697	3.9256448
N	N3	-1.2712587	-0.6997998	-0.6383205
C	C7	0.5049899	-0.3000150	-0.6399226
C	C8	0.6395050	0.9253108	-0.7786312
H	H27	-1.7223315	0.1265771	-0.9843548
H	H29	0.0426096	1.2134859	4.5550964

Total energy: 52.467 kcal/mol

One imaginary vibration: i245.44 cm⁻¹

g) (zwitter ion + MeOH $\rightarrow$ **5a** + MeOH)[‡] (stationary point, proton migration):

Cartesian Coordinates (Angstroms)

Atom Label		X	Y	Z
-----		-----	-----	-----
H	H1	1.5570208	-1.8314533	-1.0477760
C	C1	1.5650310	-0.8850575	-1.6012439
C	C2	1.6082133	1.5304264	-2.9899578
C	C3	0.8589207	0.2155401	-1.1091068
C	C4	2.2873574	-0.7718371	-2.7841902
C	C5	2.3094514	0.4328577	-3.4789138
C	C6	0.8851901	1.4253693	-1.8079887
H	H3	2.8441409	-1.6338474	-3.1656663
H	H4	2.8817521	0.5188341	-4.4084901
H	H5	0.3312565	2.2917978	-1.4164050
H	H6	1.6291370	2.4802263	-3.5337016
C	C9	1.6778145	-0.3057876	2.1170991
C	C10	2.4763061	0.7082991	2.6196476
C	C11	3.5701386	0.2199130	3.3716283
C	C12	3.6027703	-1.1649657	3.4431990
S	S1	2.2623362	-1.8747561	2.5709797
H	H10	2.2932874	1.7694348	2.4496299
H	H13	4.3089979	0.8773887	3.8399660
N	N1	4.6513465	-1.9020032	4.1681415
O	O1	5.5198857	-1.2748506	4.7481015
O	O2	4.6464112	-3.1177757	4.1860944
H	H2	-2.3050012	2.0132225	0.8454856
C	C13	-1.9515266	1.5435287	-0.0946784
C	C15	-2.1168580	-0.8562535	-0.5073056
C	C16	-3.3697014	-0.1925670	-1.0686571
C	C17	-3.0905124	1.3063590	-1.0816671
H	H7	-1.1707505	2.2185943	-0.5135074
H	H11	-1.4780545	-1.2781824	-1.3103199
H	H12	-2.3538001	-1.6929860	0.1772813
H	H14	-4.2540440	-0.4262734	-0.4452439
H	H15	-3.6098324	-0.5743812	-2.0776688
H	H16	-3.9880092	1.8921865	-0.8113488
H	H17	-2.8079050	1.6482980	-2.0959379
N	N2	-1.3569400	0.2010429	0.2527673
H	H18	-1.1441668	-0.0109571	1.5107898
C	C7	0.1340868	0.1007196	0.1500464
C	C19	0.4774408	-0.1213552	1.4091728
O	O3	-1.8930808	-0.1146326	3.1106646
C	C8	-2.1167753	1.1283049	3.7143284
H	H9	-1.4250987	1.8957265	3.3423852
H	H19	-2.0384520	1.0643838	4.8060123
H	H20	-3.1405298	1.3934454	3.4339957
H	H21	-0.9878890	-0.3705314	3.2827124

Total energy: 58.206 kcal/mol

One imaginary vibration: i1514.64 cm⁻¹

3. Transition state geometries and energies of the aminovinylation of **3g** with pyrrolidine in the presence of one molecule of methanol (PM3)

a) **3g** + pyrrolidine + MeOH (educts):

Cartesian Coordinates (Angstroms)				
Atom Label		X	Y	Z

H	H1	-1.6136797	-1.8595599	1.4640019
C	C1	-2.3645507	-1.5075501	2.1889957
C	C2	-4.2681517	-0.6119717	4.0206135
C	C3	-2.6745530	-0.1452922	2.2733629
C	C4	-3.0103955	-2.4118126	3.0231379
C	C5	-3.9602981	-1.9664748	3.9375104
C	C6	-3.6296226	0.3032518	3.1919992
H	H3	-2.7701157	-3.4783633	2.9590896
H	H4	-4.4666232	-2.6833438	4.5924279
H	H5	-3.8713871	1.3694820	3.2564554
H	H6	-5.0163919	-0.2644180	4.7408375
N	N1	1.2688836	5.0495082	-2.8735534
O	O1	2.1441440	4.6021609	-3.5896950
O	O2	0.9651921	6.2253216	-2.9157035
H	H2	1.0354677	-0.5857405	-0.1177525
C	C13	1.4806303	-1.5851342	-0.3129762
C	C15	2.5378884	-3.3406354	0.9301443
C	C16	1.1330964	-3.8381686	0.5815541
C	C17	0.4556556	-2.7140104	-0.2008554
H	H7	1.9218918	-1.5259667	-1.3336607
H	H11	3.3079500	-3.8299878	0.3037374
H	H12	2.8129557	-3.5466211	1.9811326
H	H14	0.5576630	-4.0903283	1.4920229
H	H15	1.1763007	-4.7730369	-0.0061838
H	H16	-0.4663771	-2.3690929	0.3159987
H	H17	0.1226315	-3.0527251	-1.1984006
H	H8	3.9773354	-0.0479084	-3.5847342
C	C14	2.9020689	0.0790711	-3.4132943
H	H18	2.7134110	1.1012135	-3.0446129
H	H20	2.5615657	-0.6441050	-2.6578431
O	O3	2.1430462	-0.2135024	-4.5459798
N	N3	2.5924655	-1.8837592	0.6298701
C	C7	-2.0181021	0.7766923	1.4238479
C	C8	-1.4564781	1.5433818	0.6986853
H	H27	2.4861772	-1.3539595	1.4674912
H	H29	2.4232102	0.3748731	-5.2356513
C	C9	-0.7803632	2.4257359	-0.1751433
C	C10	0.5560863	4.1368823	-1.9277354
C	C11	-1.1830280	3.7606954	-0.2922130
C	C12	0.2970176	1.9525476	-0.9328778
C	C18	0.9595801	2.8015988	-1.8064589
C	C19	-0.5171583	4.6120896	-1.1631656
H	H26	-2.0249412	4.1336634	0.3018760
H	H28	0.6197925	0.9024488	-0.8371781
H	H30	1.8001476	2.4007658	-2.4035450
H	H31	-0.8425833	5.6588918	-1.2455537

Total energy: 16.225 kcal/mol

b) phenyl nitrophenyl enamine + MeOH (products):

Cartesian Coordinates (Angstroms)				
Atom Label		X	Y	Z

H	H1	-2.2605856	-0.1008821	2.4745784
C	C1	-2.3888558	-0.8476736	1.6827909
C	C2	-2.7208200	-2.7395943	-0.3362376
C	C3	-1.7086880	-0.7045905	0.4709722
C	C4	-3.2299470	-1.9378156	1.8782510
C	C5	-3.3965672	-2.8829108	0.8711290
C	C6	-1.8773173	-1.6529920	-0.5403033
H	H3	-3.7623494	-2.0506422	2.8285983
H	H4	-4.0590467	-3.7403057	1.0291857
H	H5	-1.3411955	-1.5422341	-1.4893172
H	H6	-2.8508743	-3.4840337	-1.1287077
C	C18	0.5314645	0.3836427	0.3137657
N	N1	3.8950435	-4.0882342	1.6264065
O	O1	3.5044952	-4.9479407	2.3933124
O	O2	4.9997305	-4.1612400	1.1216865
H	H2	-0.5891558	3.4965923	0.6430767
C	C13	-0.7155079	2.9202397	-0.2931990
C	C15	-2.7437680	1.6743150	-0.7956990
C	C16	-2.6033492	2.7740419	-1.8433176
C	C17	-1.5003975	3.7007635	-1.3444616
H	H7	0.3129550	2.6718266	-0.6430631
H	H11	-2.9207046	0.6801140	-1.2531366
H	H12	-3.5966111	1.8632106	-0.1154436
H	H14	-3.5563601	3.3129599	-1.9924411
H	H15	-2.3469601	2.3485348	-2.8320912
H	H16	-1.9262637	4.6250398	-0.9099980
H	H17	-0.8456714	4.0370301	-2.1690828
H	H8	3.0532759	1.9416769	-2.6833413
C	C14	3.1919118	2.2182228	-1.6311256
H	H18	4.2428574	2.0688792	-1.3551985
H	H20	2.5555550	1.5730967	-0.9976836
O	O3	2.7522695	3.5157095	-1.3684118
H	H19	3.2996601	4.1086779	-1.8670027
H	H22	1.1382247	1.2742445	0.0410377
C	C19	-0.8184635	0.4562206	0.2508361
N	N2	-1.5049412	1.6975976	0.0416445
C	C7	1.3352879	-0.7733900	0.6683418
C	C8	3.0104940	-2.9338533	1.2991060
C	C9	0.9420095	-1.7248953	1.6141163
C	C10	2.5930739	-0.9070752	0.0590964
C	C11	3.4203946	-1.9740388	0.3626776
C	C12	1.7667857	-2.7957233	1.9270375
H	H28	-0.0311951	-1.6244750	2.1135068
H	H29	2.9215685	-0.1384771	-0.6600349
H	H30	4.3971889	-2.0583254	-0.1334116
H	H31	1.4313651	-3.5312935	2.6715555

Total energy: -7.273 kcal/mol

c) zwitter ion + MeOH (intermediate):

Cartesian Coordinates (Angstroms)				
Atom Label		X	Y	Z

H	H1	2.1696138	-1.3750848	-0.5242101
C	C1	1.5700364	-0.8687280	-1.2898919
C	C2	0.0817634	0.4816978	-3.2184690
C	C3	0.4387585	-0.1399790	-0.9124678
C	C4	1.9478674	-0.9225379	-2.6268562
C	C5	1.2045619	-0.2500259	-3.5914360
C	C6	-0.3008764	0.5389774	-1.8836072
H	H3	2.8381557	-1.4896608	-2.9187070
H	H4	1.5072636	-0.2904266	-4.6430229
H	H5	-1.1847734	1.1213924	-1.5856020
H	H6	-0.4979116	1.0198387	-3.9756880
N	N1	5.3192745	3.9331979	1.8199959
O	O1	5.2013473	5.1437219	1.7466562
O	O2	6.4189960	3.4347503	1.9835539
H	H2	-2.8518518	0.4440012	1.2761400
C	C13	-2.4302905	-0.2327846	0.5037418
C	C15	-1.1013005	-2.2732000	0.5987284
C	C16	-2.5592505	-2.6867021	0.4387939
C	C17	-3.3535399	-1.4068657	0.1896091
H	H7	-2.2561547	0.4074759	-0.3941150
H	H11	-0.5297507	-2.4020869	-0.3468335
H	H12	-0.5674704	-2.8785811	1.3588536
H	H14	-2.9238161	-3.2122464	1.3426340
H	H15	-2.6771357	-3.4097686	-0.3890346
H	H16	-4.2681855	-1.3751213	0.8108329
H	H17	-3.7079321	-1.3528248	-0.8571839
N	N2	-1.1086063	-0.8075743	0.9977975
H	H18	-1.0966321	-0.7306149	2.0331147
C	C7	0.0899812	-0.0470718	0.5104744
C	C19	0.7068985	0.6023257	1.4842951
O	O3	-0.6034299	-0.1266326	3.6371002
C	C8	-1.3877281	0.8316613	4.2692271
H	H9	-2.0215256	1.3690723	3.5496733
H	H19	-0.7805145	1.5587324	4.8209022
H	H20	-2.0257369	0.2856550	4.9705512
H	H21	0.0540635	0.3192250	3.0326005
C	C9	1.8617071	1.4247970	1.4934225
C	C10	4.1233477	3.0653791	1.7068841
C	C11	3.1329427	0.8611363	1.6965515
C	C12	1.7393716	2.8208968	1.3927771
C	C14	2.8550161	3.6303312	1.4986634
C	C18	4.2483207	1.6703318	1.8048512
H	H28	3.2331996	-0.2271629	1.7688743
H	H29	0.7522076	3.2654238	1.2300548
H	H30	2.7387821	4.7197260	1.4175185
H	H31	5.2330026	1.2106904	1.9660477

Total energy: 34.382 kcal/mol

d) (**3g** + pyrrolidine + MeOH $\rightarrow$ zwitter ion + MeOH)[‡] (stationary point, amine addition):

Cartesian Coordinates (Angstroms)

Atom Label		X	Y	Z
-----		-----	-----	-----
H	H1	-1.1643468	-3.6025180	1.1136755
C	C1	-1.1252991	-2.9268912	1.9754073
C	C2	-1.0538602	-1.1991432	4.1627868
C	C3	-0.8815700	-1.5631218	1.7820917
C	C4	-1.3347576	-3.4165805	3.2597109
C	C5	-1.3015277	-2.5554696	4.3520977
C	C6	-0.8427050	-0.7012773	2.8828987
H	H3	-1.5315933	-4.4835814	3.4097853
H	H4	-1.4723033	-2.9447933	5.3611971
H	H5	-0.6326221	0.3672275	2.7250657
H	H6	-1.0284326	-0.5215100	5.0226660
N	N1	-4.4597206	0.3338278	-5.2303068
O	O1	-4.9351099	1.4443524	-5.3868340
O	O2	-4.6337507	-0.5325610	-6.0687570
H	H2	1.2010096	1.5194307	0.0804884
C	C13	1.3753711	0.6953653	0.7992680
C	C15	2.0060252	-1.6332707	0.7047220
C	C16	3.2192512	-0.8640311	1.2238431
C	C17	2.8289707	0.6124632	1.2586062
H	H7	0.6820422	0.8724015	1.6539051
H	H11	1.5120763	-2.2134678	1.5114239
H	H12	2.2731651	-2.3635856	-0.0825160
H	H14	4.1017878	-1.0271150	0.5776416
H	H15	3.5177034	-1.2278246	2.2240181
H	H16	3.4887763	1.2138940	0.6051200
H	H17	2.9491686	1.0414252	2.2703877
N	N2	1.0185914	-0.6289985	0.1807201
H	H18	1.1158591	-0.5580515	-0.8317377
C	C7	-0.7564103	-1.0485854	0.4371497
C	C19	-1.3800777	-0.7892536	-0.5991476
O	O3	1.1088344	-0.5076128	-2.6694414
C	C8	1.4022799	0.7503100	-3.2068374
H	H9	0.8981050	1.5518831	-2.6505030
H	H19	1.1351349	0.8192931	-4.2679707
H	H20	2.4856685	0.8535134	-3.0946481
H	H21	0.1830708	-0.6822476	-2.8261490
C	C9	-2.1435567	-0.5183596	-1.7247076
C	C10	-3.6585059	0.0386975	-4.0188026
C	C11	-2.2493484	-1.4690494	-2.7605668
C	C12	-2.8078849	0.7175863	-1.8599320
C	C14	-3.5543642	0.9893574	-2.9892962
C	C18	-3.0026868	-1.1956337	-3.8860346
H	H28	-1.7479774	-2.4375646	-2.6578552
H	H29	-2.7381539	1.4577472	-1.0560497
H	H30	-4.0683213	1.9568924	-3.0743478
H	H31	-3.0829209	-1.9547480	-4.6765422

Total energy: 42.782 kcal/mol

One imaginary vibration: i232.80 cm⁻¹

e) (zwitter ion + MeOH $\rightarrow$ phenyl nitrophenyl enamine + MeOH)[‡] (stationary point, proton migration):

Cartesian Coordinates (Angstroms)				
Atom Label		X	Y	Z

H	H1	1.0360301	-2.1589289	-0.4170124
C	C1	0.8420459	-1.5424826	-1.3031658
C	C2	0.3896109	0.0519645	-3.5411778
C	C3	0.3045383	-0.2612352	-1.1489229
C	C4	1.1454483	-2.0209681	-2.5726961
C	C5	0.9186828	-1.2264872	-3.6920084
C	C6	0.0834636	0.5358102	-2.2746309
H	H3	1.5670599	-3.0247606	-2.6900323
H	H4	1.1600102	-1.6053628	-4.6904626
H	H5	-0.3312284	1.5476191	-2.1547466
H	H6	0.2184237	0.6808765	-4.4210580
N	N1	6.1768622	-0.0841127	2.9256730
O	O1	6.8640821	0.9138480	3.0486195
O	O2	6.6394815	-1.1837679	3.1697794
H	H2	-1.7707787	2.6823094	0.7034156
C	C13	-1.9645093	1.8135372	0.0442950
C	C15	-2.3768574	-0.5286509	0.5922206
C	C16	-3.6141689	0.0243113	-0.1094093
C	C17	-3.4532666	1.5402771	-0.1370977
H	H7	-1.4637991	2.0365569	-0.9259039
H	H11	-1.9538906	-1.4057588	0.0628400
H	H12	-2.6019499	-0.8627186	1.6238928
H	H14	-4.5418171	-0.2793352	0.4091030
H	H15	-3.7009772	-0.3839591	-1.1345400
H	H16	-4.0437349	2.0173172	0.6680412
H	H17	-3.8311268	1.9763950	-1.0796550
N	N2	-1.3584237	0.5808668	0.6697137
H	H18	-0.7717263	0.7628233	1.7973970
C	C7	0.0169683	0.2241340	0.1943200
C	C19	0.7355322	0.4158686	1.2897405
O	O3	-0.9152270	1.0959104	3.5470526
C	C8	-1.0840743	2.4395545	3.8944538
H	H9	-0.8659917	3.1046688	3.0479050
H	H19	-0.4609187	2.7247230	4.7502283
H	H20	-2.1402716	2.5284288	4.1652421
H	H21	0.0154415	0.9412214	3.3778387
C	C9	2.1060130	0.2771161	1.6346164
C	C10	4.7664835	0.0409879	2.4768155
C	C11	2.6325603	-0.9770979	1.9794831
C	C12	2.9298915	1.4110791	1.7099684
C	C14	4.2449092	1.2951535	2.1253204
C	C18	3.9465529	-1.0949873	2.3969678
H	H28	1.9950716	-1.8664199	1.9104662
H	H29	2.5266480	2.3904619	1.4316780
H	H30	4.8747669	2.1944238	2.1767323
H	H31	4.3402231	-2.0864541	2.6624959

Total energy: 46.730 kcal/mol

One imaginary vibration: i1466.36 cm⁻¹

4. Equilibrium geometries of the structures **5** (AM1)

Compound **5a**:

Cartesian Coordinates (Angstroms)				
Atom Label		X	Y	Z

H	H1	-0.8378310	1.8420099	0.7589658
C	C1	-0.6114832	0.9967674	1.4294572
C	C2	0.0510429	-1.0905662	3.1653075
C	C3	0.1360412	-0.0937458	0.9615539
C	C4	-1.0143688	1.0407226	2.7664237
C	C5	-0.6880963	-0.0025608	3.6318175
C	C6	0.4673834	-1.1371333	1.8360642
H	H3	-1.5963367	1.9002342	3.1322915
H	H4	-1.0150147	0.0315287	4.6819875
H	H5	1.0541320	-1.9924298	1.4671420
H	H6	0.3067256	-1.9151469	3.8475013
C	C9	-1.7490243	-0.4511643	-1.2721031
C	C10	-2.6121648	-0.9341199	-2.2610005
C	C11	-3.9597737	-0.9372131	-1.8400861
C	C12	-4.0815382	-0.4467699	-0.5356861
S	S1	-2.5829199	-0.0189276	0.1101957
H	H10	-2.2864190	-1.2761229	-3.2453079
H	H13	-4.8009636	-1.2791247	-2.4516653
N	N1	-5.3477097	-0.3288729	0.1639627
O	O1	-6.3602328	-0.6794468	-0.3845831
O	O2	-5.3618390	0.1224481	1.2824473
C	C13	0.5770053	-0.1474377	-0.4534537
N	N2	1.9525450	-0.1325536	-0.6873580
C	C15	2.8492881	0.4173478	0.3244483
C	C16	4.0871065	0.9819887	-0.3890455
C	C17	3.8485785	0.7927062	-1.8823789
C	C18	2.4491126	0.1743695	-2.0236467
H	H20	3.1343071	-0.4191596	1.0204763
H	H21	2.3463808	1.2176786	0.9348070
H	H22	4.2198382	2.0625825	-0.1365083
H	H23	5.0048995	0.4374185	-0.0586137
H	H24	4.6173003	0.1135821	-2.3256332
H	H25	3.8976789	1.7671718	-2.4261604
H	H26	2.4888523	-0.7843619	-2.6094976
H	H27	1.7641293	0.8852327	-2.5660876
C	C19	-0.3377967	-0.3188333	-1.4574402
H	H32	-0.0088351	-0.3980986	-2.5085933

Total energy: 74.572 kcal/mol

Compound **5d**:

Cartesian Coordinates (Angstroms)				
Atom Label		X	Y	Z

H	H1	1.2319732	-0.9529184	-1.8892899
C	C1	0.2340053	-1.2303338	-1.5149026
C	C2	-2.3257787	-1.8823618	-0.6027178
C	C3	-0.2220767	-0.7275059	-0.2874829
C	C4	-0.5989015	-2.0450963	-2.2848752

C	C5	-1.8760613	-2.3716236	-1.8297882
C	C6	-1.5047853	-1.0606417	0.1681008
H	H3	-0.2411877	-2.4325214	-3.2509126
H	H4	-2.5274583	-3.0179751	-2.4371431
H	H5	-1.8561305	-0.6785568	1.1389356
H	H6	-3.3308108	-2.1455519	-0.2404146
C	C9	1.9805079	-1.8000497	1.2763712
C	C10	2.8361006	-2.3940101	2.2091670
C	C11	3.0149583	-3.7733803	1.9663439
C	C12	2.2880501	-4.1862336	0.8444535
S	S1	1.4313605	-2.9083764	0.1521477
H	H10	3.3115343	-1.8591371	3.0338623
H	H13	3.6389013	-4.4356865	2.5750798
N	N1	2.2781062	-5.5515014	0.3511823
O	O1	2.9137074	-6.3932227	0.9312479
O	O2	1.6338715	-5.8165352	-0.6335519
C	C13	0.6507664	0.1518284	0.5296475
N	N2	0.3395042	1.5127785	0.5909657
C	C15	-0.4566897	2.1299295	-0.4798080
C	C16	0.1957058	3.4861815	-0.8262970
C	C17	1.2111653	3.7628176	0.2725120
C	C18	1.3749022	2.4419272	1.0385007
C	C7	-1.9170956	2.3411585	-0.0295781
H	H21	-0.4770776	1.4730534	-1.3974559
H	H22	0.6962274	3.4188924	-1.8236009
H	H23	-0.5805331	4.2874462	-0.8870375
H	H24	0.8460492	4.5652732	0.9597031
H	H25	2.1904480	4.0928877	-0.1508763
H	H26	1.2448072	2.5972895	2.1441635
H	H27	2.4065733	2.0254560	0.8625822
C	C19	1.6576166	-0.4072111	1.2711014
H	H32	2.2836083	0.2096918	1.9389551
H	H2	-1.9824235	3.0773419	0.8134112
H	H7	-2.3814399	1.3683475	0.2836346
O	O3	-2.6025652	2.8568363	-1.1700214
C	C8	-3.9893201	3.0293655	-0.9324454
H	H11	-4.1596986	3.7511769	-0.0957361
H	H12	-4.4735965	2.0501205	-0.6944107
H	H14	-4.3868196	3.4406302	-1.8937220

Total energy: 31.145 kcal/mol

Compound 5e:

Cartesian Coordinates (Angstroms)

Atom Label		X	Y	Z
-----		-----	-----	-----
C	C9	-0.1350524	-2.2860007	-0.5061757
C	C10	-0.1383286	-3.5316096	-1.1497867
C	C11	0.1597563	-4.5943732	-0.2726703
C	C12	0.3880288	-4.1289297	1.0265106
S	S1	0.2376552	-2.4508338	1.1164954
H	H10	-0.3528481	-3.6688086	-2.2117021
H	H13	0.2045662	-5.6487294	-0.5649354
N	N1	0.7095410	-4.9882170	2.1498298
O	O1	0.8060414	-6.1751027	1.9744759
O	O2	0.8749022	-4.4956664	3.2384648
C	C13	-0.6577295	0.1676200	-0.6745210
N	N2	-0.9873252	1.2384141	-1.4940614

C	C15	-1.0298464	2.6053847	-0.9986342
C	C16	-0.8450117	3.5502096	-2.1973385
C	C17	-0.6672264	2.6632662	-3.4239469
C	C18	-0.6867415	1.2126743	-2.9175452
H	H20	-0.2318817	2.7920410	-0.2276987
H	H21	-2.0303916	2.7760573	-0.5125178
H	H22	-1.7375926	4.2129961	-2.3075668
H	H23	0.0489672	4.2018754	-2.0403878
H	H24	0.2990577	2.8793240	-3.9412758
H	H25	-1.4936567	2.8271491	-4.1580270
H	H26	0.3055526	0.7169531	-3.1138865
H	H27	-1.4836148	0.6153048	-3.4403641
C	C19	-0.3892225	-1.0698746	-1.2056686
H	H32	-0.3883831	-1.2024850	-2.3044135
C	C1	-0.7100561	0.3839767	0.8160076
C	C2	0.6613323	0.6941433	1.3868884
H	H16	-1.1275932	-0.5420996	1.3050987
H	H17	-1.4207769	1.2135849	1.0809578
H	H18	1.1285643	1.5452103	0.8255299
H	H19	1.3349549	-0.1964808	1.2547287
C	C3	0.5696616	1.0465331	2.8571989
C	C4	1.9315701	1.3175935	3.4423087
H	H30	0.0806144	0.2042214	3.4147904
H	H31	-0.0828310	1.9506315	2.9849504
H	H33	2.5849959	0.4158184	3.3558583
H	H34	1.8408401	1.5843962	4.5229608
H	H35	2.4295077	2.1638321	2.9100690

Total energy: 21.533 kcal/mol

Compound 5g:

Cartesian Coordinates (Angstroms)

Atom Label	X	Y	Z

H H1	-2.1149194	-1.4343688	0.4909219
C C1	-1.4488290	-0.9337349	1.2105503
C C2	0.2380455	0.3514573	3.0302631
C C3	-0.4190211	-0.1053521	0.7441810
C C4	-1.6239134	-1.1219670	2.5804416
C C5	-0.7831272	-0.4791530	3.4903839
C C6	0.4287760	0.5371674	1.6587451
H H3	-2.4285489	-1.7790041	2.9436105
H H4	-0.9248540	-0.6287581	4.5715159
H H5	1.2135873	1.2226011	1.3002417
H H6	0.9011307	0.8604385	3.7463622
C C9	1.8111070	-1.2720906	-0.7633806
N N3	2.7019870	-2.0106089	-1.4779858
C C11	3.5511152	-2.6584474	-0.6315598
C C12	3.3204741	-2.4185562	0.7395015
S S1	2.0147090	-1.3640638	0.9337692
H H13	4.3402360	-3.3103104	-1.0344795
N N1	4.1069857	-3.0091403	1.8014035
O O1	5.0076169	-3.7568021	1.5194491
O O2	3.8467995	-2.7391178	2.9474025
C C13	-0.2487277	0.1092689	-0.7145711
N N2	-1.2527873	0.8121943	-1.3660732
C C15	-2.1525336	1.6816852	-0.6175136
C C16	-2.6504464	2.7806652	-1.5687509

C	C17	-1.9747839	2.5298558	-2.9120792
C	C18	-1.0347357	1.3313874	-2.7101260
H	H20	-1.6390219	2.1331108	0.2760940
H	H21	-3.0090846	1.0552547	-0.2442289
H	H22	-3.7625721	2.7338725	-1.6646104
H	H23	-2.3829863	3.7885505	-1.1672128
H	H24	-1.3943889	3.4244931	-3.2449494
H	H25	-2.7309782	2.2982174	-3.7015925
H	H26	0.0366007	1.6460558	-2.8584908
H	H27	-1.2612229	0.5110232	-3.4451920
C	C19	0.8052769	-0.4565667	-1.3849320
H	H32	0.9130347	-0.3292570	-2.4771087

Total energy: 87.880 kcal/mol

II. ^1H NMR spectra

III. X-Ray structure data of enamine 5e

ORTEP plot of compound **5e**. Selected bond lengths [Å]: N(2)-C(7) 1.348(3), C(6)-C(7) 1.382(4), C(5)-C(6) 1.413(4), C(4)-C(5) 1.396(4), C(3)-C(4) 1.370(4), C(2)-C(3) 1.372(4), C(2)-N(1) 1.387(5).

Table 1: Crystal data and structure refinement for **5e**.

Identification code	aka1
Empirical formula	C ₁₄ H ₂₀ N ₂ O ₂ S
Formula weight	280.38
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /n
Z	12
Unit cell dimensions	a = 12.4935(4) Å α = 90 deg. b = 17.5289(5) Å β = 99.065(1) deg. c = 19.9857(5) Å γ = 90 deg.
Volume	4322.1(2) Å ³
Density (calculated)	1.29 g/cm ³
Absorption coefficient	0.22 mm ⁻¹
Crystal shape	needle
Crystal size	0.54 x 0.16 x 0.09 mm ³
Theta range for data collection	1.5 to 24.1 deg.
Index ranges	-14 ≤ h ≤ 14, -20 ≤ k ≤ 20, -22 ≤ l ≤ 22
Reflections collected	33915
Independent reflections	6872 (R(int) = 0.0682)
Observed reflections	3787 (I > 2σ(I))

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9801 and 0.8882
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	6872 / 1 / 512
Goodness-of-fit on F^2	1.01
Final R indices ($I > 2\sigma(I)$)	$R1 = 0.047$, $wR2 = 0.101$
Largest diff. peak and hole	0.38 and $-0.35 \text{ e}\text{\AA}^{-3}$

Table 2: Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2$) for 5e. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
S11	0.6028(1)	0.7898(1)	0.1750(1)	0.0517(2)
N11	0.5388(3)	0.9374(2)	0.1717(1)	0.0693(9)
O11	0.4688(2)	0.9884(1)	0.1727(1)	0.0904(9)
O21	0.6360(2)	0.9509(1)	0.1683(1)	0.0852(8)
N21	0.6036(2)	0.5191(1)	0.1777(1)	0.0475(6)
C21	0.5074(3)	0.8609(2)	0.1741(1)	0.0529(8)
C31	0.4052(3)	0.8336(2)	0.1744(1)	0.0568(9)
C41	0.4032(2)	0.7552(2)	0.1747(1)	0.0522(8)
C51	0.5039(2)	0.7201(2)	0.1748(1)	0.0441(8)
C61	0.5172(2)	0.6396(2)	0.1745(1)	0.0443(7)
C71	0.6101(2)	0.5959(2)	0.1801(1)	0.0443(8)
C81	0.7222(2)	0.6291(2)	0.1928(1)	0.0450(8)
C91	0.7630(2)	0.6412(2)	0.2685(1)	0.0455(8)
C101	0.8792(2)	0.6684(2)	0.2825(2)	0.0555(9)
C111	0.9216(2)	0.6753(2)	0.3578(2)	0.0685(10)
C121	0.5003(2)	0.4775(2)	0.1656(2)	0.0581(9)
C131	0.5351(3)	0.3941(2)	0.1655(2)	0.0725(11)
C141	0.6445(3)	0.3932(2)	0.2100(2)	0.0671(10)
C151	0.6960(2)	0.4663(2)	0.1906(2)	0.0554(9)
S12	0.0621(1)	0.1687(1)	0.1582(1)	0.0540(3)
N12	0.1066(3)	0.0180(2)	0.1642(2)	0.0839(11)
O12	0.1696(3)	-0.0376(2)	0.1664(1)	0.1137(11)
O22	0.0075(3)	0.0106(2)	0.1650(1)	0.0969(10)
N22	0.0992(2)	0.4375(2)	0.1546(1)	0.0554(7)
C22	0.1475(3)	0.0913(2)	0.1614(2)	0.0638(10)
C32	0.2538(3)	0.1115(2)	0.1625(2)	0.0716(11)
C42	0.2664(3)	0.1891(2)	0.1615(2)	0.0631(9)
C52	0.1707(2)	0.2307(2)	0.1597(1)	0.0465(8)
C62	0.1681(2)	0.3113(2)	0.1590(1)	0.0482(8)
C72	0.0825(2)	0.3614(2)	0.1554(1)	0.0454(8)
C82	-0.0330(2)	0.3354(2)	0.1486(1)	0.0458(8)
C92	-0.0833(2)	0.3228(2)	0.0742(1)	0.0447(8)
C102	-0.1992(2)	0.2955(2)	0.0664(2)	0.0507(8)
C112	-0.2519(2)	0.2867(2)	-0.0065(2)	0.0580(9)
C122	0.2084(3)	0.4708(2)	0.1584(2)	0.0714(11)
C132	0.1870(3)	0.5561(2)	0.1544(2)	0.0915(12)
C142	0.0700(3)	0.5646(2)	0.1228(2)	0.1001(14)
C152	0.0151(3)	0.4963(2)	0.1482(2)	0.0693(10)
S13	0.7750(1)	0.6751(1)	0.0153(1)	0.0504(2)
N13	0.7205(3)	0.5259(2)	0.0154(1)	0.0639(8)
O13	0.6542(2)	0.4721(1)	0.0126(1)	0.0790(8)
O23	0.8204(2)	0.5149(1)	0.0194(1)	0.0853(8)
N23	0.7563(2)	0.9444(1)	0.0084(1)	0.0475(6)
C23	0.6844(3)	0.6008(2)	0.0130(1)	0.0490(8)
C33	0.5793(2)	0.6245(2)	0.0092(1)	0.0533(8)

C43	0.5715(2)	0.7027(2)	0.0071(2)	0.0523(8)
C53	0.6703(2)	0.7412(2)	0.0096(1)	0.0432(8)
C63	0.6781(2)	0.8217(2)	0.0082(1)	0.0467(8)
C73	0.7672(2)	0.8683(2)	0.0123(1)	0.0435(8)
C83	0.8812(2)	0.8382(2)	0.0232(1)	0.0440(8)
C93	0.9244(2)	0.8244(2)	0.0984(1)	0.0409(7)
C103	1.0393(2)	0.7939(2)	0.1094(2)	0.0520(8)
C113	1.0842(2)	0.7805(2)	0.1834(2)	0.0680(10)
C123	0.6502(2)	0.9833(2)	-0.0025(2)	0.0599(9)
C133	0.6797(3)	1.0662(2)	-0.0111(2)	0.0748(11)
C143	0.7903(3)	1.0741(2)	0.0320(2)	0.0736(11)
C153	0.8456(3)	1.0004(2)	0.0182(2)	0.0572(9)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2$) for 5e.

Atom	x	y	z	U_{eq}
H31	0.3431	0.8649	0.1745	0.068
H41	0.3383	0.7270	0.1747	0.063
H61	0.4515	0.6114	0.1698	0.053
H8A1	0.7221	0.6786	0.1689	0.054
H8B1	0.7724	0.5945	0.1739	0.054
H9A1	0.7161	0.6792	0.2864	0.055
H9B1	0.7569	0.5926	0.2928	0.055
H10A1	0.8844	0.7187	0.2607	0.067
H10B1	0.9254	0.6322	0.2619	0.067
H11A1	0.8752	0.7103	0.3786	0.103
H11B1	0.9958	0.6951	0.3643	0.103
H11C1	0.9210	0.6250	0.3791	0.103
H12A1	0.4573	0.4920	0.1215	0.070
H12B1	0.4568	0.4875	0.2020	0.070
H13A1	0.4831	0.3609	0.1845	0.087
H13B1	0.5406	0.3766	0.1191	0.087
H14A1	0.6874	0.3482	0.2003	0.081
H14B1	0.6371	0.3932	0.2585	0.081
H15A1	0.7514	0.4849	0.2280	0.066
H15B1	0.7300	0.4592	0.1496	0.066
H32	0.3116	0.0761	0.1637	0.086
H42	0.3349	0.2128	0.1620	0.076
H62	0.2371	0.3349	0.1614	0.058
H8A2	-0.0758	0.3742	0.1689	0.055
H8B2	-0.0362	0.2872	0.1740	0.055
H9A2	-0.0808	0.3713	0.0491	0.054
H9B2	-0.0395	0.2848	0.0539	0.054
H10A2	-0.2419	0.3322	0.0891	0.061
H10B2	-0.2009	0.2457	0.0897	0.061
H11A2	-0.2581	0.3367	-0.0286	0.087
H11B2	-0.3243	0.2645	-0.0082	0.087
H11C2	-0.2077	0.2530	-0.0302	0.087
H12A2	0.2439	0.4534	0.1202	0.086
H12B2	0.2548	0.4571	0.2016	0.086
H13A2	0.1997	0.5791	0.2002	0.110
H13B2	0.2350	0.5813	0.1262	0.110
H14A2	0.0391	0.6127	0.1374	0.120
H14B2	0.0622	0.5642	0.0727	0.120
H15A2	-0.0077	0.5071	0.1925	0.083
H15B2	-0.0491	0.4808	0.1155	0.083
H33	0.5192	0.5911	0.0081	0.064

H43	0.5042	0.7286	0.0042	0.063
H63	0.6107	0.8477	0.0037	0.056
H8A3	0.9289	0.8751	0.0048	0.053
H8B3	0.8833	0.7897	-0.0019	0.053
H9A3	0.9224	0.8730	0.1235	0.049
H9B3	0.8766	0.7876	0.1169	0.049
H10A3	1.0409	0.7452	0.0844	0.062
H10B3	1.0867	0.8306	0.0903	0.062
H11A3	1.0836	0.8285	0.2084	0.102
H11B3	1.1588	0.7616	0.1874	0.102
H11C3	1.0394	0.7427	0.2022	0.102
H12A3	0.6122	0.9766	0.0369	0.072
H12B3	0.6036	0.9638	-0.0436	0.072
H13A3	0.6264	1.1005	0.0052	0.090
H13B3	0.6830	1.0780	-0.0592	0.090
H14A3	0.8299	1.1188	0.0180	0.088
H14B3	0.7843	1.0790	0.0806	0.088
H15A3	0.8801	1.0047	-0.0230	0.069
H15B3	0.9013	0.9861	0.0570	0.069

Table 4: Anisotropic displacement parameters ($\text{\AA}^2$) for 5e. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 (h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12})$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S11	0.0565(5)	0.0486(5)	0.0485(5)	-0.0028(4)	0.0036(4)	-0.0029(4)
N11	0.090(3)	0.059(2)	0.050(2)	0.0005(15)	-0.0181(18)	0.001(2)
O11	0.113(2)	0.0535(16)	0.092(2)	0.0005(13)	-0.0224(16)	0.0246(15)
O21	0.094(2)	0.0590(16)	0.091(2)	0.0028(13)	-0.0192(17)	-0.0163(15)
N21	0.0525(17)	0.0433(16)	0.0459(16)	-0.0071(12)	0.0050(12)	-0.0041(13)
C21	0.069(2)	0.046(2)	0.040(2)	0.0021(15)	-0.0048(16)	0.0031(18)
C31	0.063(2)	0.063(2)	0.041(2)	0.0048(16)	-0.0040(17)	0.0165(19)
C41	0.049(2)	0.062(2)	0.044(2)	0.0043(16)	0.0006(15)	0.0053(17)
C51	0.049(2)	0.054(2)	0.0273(18)	0.0000(14)	0.0027(14)	-0.0011(16)
C61	0.0462(19)	0.048(2)	0.0378(19)	-0.0033(14)	0.0041(14)	-0.0060(15)
C71	0.052(2)	0.053(2)	0.0284(18)	-0.0048(15)	0.0067(14)	-0.0035(17)
C81	0.0454(19)	0.0448(18)	0.047(2)	-0.0004(14)	0.0148(15)	0.0004(15)
C91	0.0433(18)	0.0481(18)	0.045(2)	-0.0025(14)	0.0072(15)	-0.0005(14)
C101	0.044(2)	0.052(2)	0.073(3)	-0.0132(17)	0.0149(18)	-0.0071(15)
C111	0.0354(19)	0.083(3)	0.084(3)	-0.023(2)	0.0019(19)	-0.0046(17)
C121	0.062(2)	0.056(2)	0.053(2)	-0.0049(16)	-0.0014(17)	-0.0134(17)
C131	0.100(3)	0.048(2)	0.064(3)	0.0014(17)	-0.006(2)	-0.018(2)
C141	0.087(3)	0.058(2)	0.056(2)	0.0022(17)	0.010(2)	-0.0005(19)
C151	0.066(2)	0.049(2)	0.052(2)	-0.0019(16)	0.0116(17)	0.0052(17)
S12	0.0636(6)	0.0538(5)	0.0429(5)	-0.0013(4)	0.0030(4)	-0.0081(4)
N12	0.136(3)	0.059(2)	0.047(2)	-0.0044(16)	-0.018(2)	-0.001(3)
O12	0.179(3)	0.0571(18)	0.092(2)	-0.0035(15)	-0.019(2)	0.0249(19)
O22	0.135(3)	0.0692(18)	0.076(2)	0.0030(14)	-0.017(2)	-0.0295(19)
N22	0.0607(19)	0.0514(18)	0.0501(18)	0.0029(13)	-0.0037(14)	-0.0164(15)
C22	0.095(3)	0.056(2)	0.036(2)	-0.0046(16)	-0.0027(19)	0.004(2)
C32	0.085(3)	0.078(3)	0.048(2)	-0.0068(19)	0.000(2)	0.026(2)
C42	0.059(2)	0.080(3)	0.048(2)	-0.0020(18)	0.0043(18)	0.007(2)
C52	0.048(2)	0.059(2)	0.0309(19)	-0.0001(15)	0.0041(15)	-0.0028(16)
C62	0.041(2)	0.066(2)	0.036(2)	0.0035(15)	0.0031(15)	-0.0120(16)
C72	0.048(2)	0.054(2)	0.0328(19)	0.0015(14)	0.0012(15)	-0.0118(17)
C82	0.049(2)	0.0460(18)	0.043(2)	-0.0014(14)	0.0104(15)	-0.0047(14)
C92	0.0439(19)	0.0487(18)	0.041(2)	0.0023(14)	0.0061(15)	-0.0037(14)
C102	0.0393(19)	0.0557(19)	0.058(2)	-0.0116(16)	0.0118(16)	-0.0011(15)

C112	0.0431(19)	0.064(2)	0.065(2)	-0.0134(17)	0.0030(17)	0.0033(16)
C122	0.075(3)	0.066(2)	0.066(3)	0.0096(18)	-0.0119(19)	-0.030(2)
C142	0.127(4)	0.050(2)	0.121(4)	0.014(2)	0.015(3)	-0.009(2)
C152	0.089(3)	0.049(2)	0.067(3)	0.0009(18)	0.004(2)	-0.002(2)
S13	0.0496(5)	0.0518(5)	0.0482(6)	-0.0001(4)	0.0033(4)	0.0043(4)
N13	0.080(2)	0.055(2)	0.0504(19)	0.0014(14)	-0.0088(17)	0.0031(18)
O13	0.0934(19)	0.0485(15)	0.0866(19)	0.0002(13)	-0.0120(15)	-0.0145(13)
O23	0.0777(19)	0.0611(16)	0.108(2)	-0.0043(14)	-0.0122(16)	0.0167(14)
N23	0.0484(16)	0.0473(16)	0.0448(17)	0.0044(12)	0.0010(12)	0.0017(13)
C23	0.060(2)	0.046(2)	0.037(2)	0.0001(14)	-0.0050(16)	-0.0001(16)
C33	0.055(2)	0.060(2)	0.043(2)	-0.0005(16)	0.0003(16)	-0.0105(17)
C43	0.043(2)	0.062(2)	0.051(2)	-0.0004(16)	0.0048(16)	0.0016(16)
C53	0.0444(19)	0.055(2)	0.0294(18)	0.0012(14)	0.0018(14)	0.0033(15)
C63	0.044(2)	0.051(2)	0.043(2)	0.0032(15)	0.0011(15)	0.0052(16)
C73	0.053(2)	0.0459(19)	0.0314(19)	0.0033(14)	0.0047(15)	0.0044(16)
C83	0.0431(19)	0.0495(19)	0.041(2)	0.0006(14)	0.0120(15)	0.0023(14)
C93	0.0373(18)	0.0443(17)	0.041(2)	-0.0001(14)	0.0070(14)	0.0020(13)
C103	0.0395(19)	0.056(2)	0.063(2)	0.0057(16)	0.0127(16)	0.0037(15)
C113	0.047(2)	0.083(3)	0.072(3)	0.021(2)	0.0011(18)	0.0067(18)
C123	0.059(2)	0.057(2)	0.060(2)	0.0051(17)	-0.0035(17)	0.0138(17)
C133	0.088(3)	0.056(2)	0.076(3)	0.0101(19)	0.001(2)	0.015(2)
C143	0.091(3)	0.048(2)	0.080(3)	0.0029(18)	0.005(2)	0.0021(19)
C153	0.064(2)	0.053(2)	0.053(2)	0.0062(16)	0.0063(17)	-0.0033(17)

Table 5: Bond lengths (Å) and angles (deg) for 5e.

S11-C21	1.723(3)
S11-C51	1.737(3)
N11-O21	1.249(3)
N11-O11	1.253(3)
N11-C21	1.399(4)
N21-C71	1.348(3)
N21-C121	1.469(3)
N21-C151	1.472(3)
C21-C31	1.365(4)
C31-C41	1.374(4)
C41-C51	1.401(4)
C51-C61	1.419(4)
C61-C71	1.382(4)
C71-C81	1.500(4)
C81-C91	1.533(3)
C91-C101	1.512(3)
C101-C111	1.520(4)
C121-C131	1.526(4)
C131-C141	1.508(4)
C141-C151	1.511(4)
S12-C22	1.722(4)
S12-C52	1.734(3)
N12-O22	1.247(4)
N12-O12	1.250(4)
N12-C22	1.387(5)
N22-C72	1.350(4)
N22-C152	1.464(4)
N22-C122	1.475(4)
C22-C32	1.372(4)
C32-C42	1.370(4)
C42-C52	1.396(4)
C52-C62	1.413(4)
C62-C72	1.377(4)
C72-C82	1.498(4)

C82-C92	1.536(4)
C92-C102	1.509(3)
C102-C112	1.511(4)
C122-C132	1.518(5)
C132-C142	1.506(5)
C142-C152	1.506(4)
S13-C23	1.722(3)
S13-C53	1.738(3)
N13-O13	1.250(3)
N13-O23	1.253(3)
N13-C23	1.387(4)
N23-C73	1.342(3)
N23-C123	1.476(3)
N23-C153	1.476(4)
C23-C33	1.368(4)
C33-C43	1.374(4)
C43-C53	1.401(4)
C53-C63	1.413(4)
C63-C73	1.373(4)
C73-C83	1.503(4)
C83-C93	1.534(3)
C93-C103	1.516(3)
C103-C113	1.515(4)
C123-C133	1.515(4)
C133-C143	1.516(4)
C143-C153	1.510(4)
C21-S11-C51	91.09(15)
O21-N11-O11	123.5(3)
O21-N11-C21	117.7(3)
O11-N11-C21	118.8(3)
C71-N21-C121	123.3(2)
C71-N21-C151	125.5(3)
C121-N21-C151	111.2(2)
C31-C21-N11	127.2(3)
C31-C21-S11	113.1(2)
N11-C21-S11	119.7(3)
C21-C31-C41	111.6(3)
C31-C41-C51	115.0(3)
C41-C51-C61	122.8(3)
C41-C51-S11	109.2(2)
C61-C51-S11	128.0(2)
C71-C61-C51	130.4(3)
N21-C71-C61	120.4(3)
N21-C71-C81	116.3(3)
C61-C71-C81	123.2(3)
C71-C81-C91	112.2(2)
C101-C91-C81	112.7(2)
C91-C101-C111	112.5(3)
N21-C121-C131	103.5(2)
C141-C131-C121	103.9(2)
C131-C141-C151	103.0(3)
N21-C151-C141	102.9(2)
C22-S12-C52	90.81(17)
O22-N12-O12	122.6(4)
O22-N12-C22	118.1(4)
O12-N12-C22	119.3(4)
C72-N22-C152	125.9(3)
C72-N22-C122	122.3(3)
C152-N22-C122	111.7(2)
C32-C22-N12	126.9(4)
C32-C22-S12	113.0(3)
N12-C22-S12	120.1(3)

C42-C32-C22	111.6(3)
C32-C42-C52	114.8(3)
C42-C52-C62	122.7(3)
C42-C52-S12	109.8(2)
C62-C52-S12	127.6(2)
C72-C62-C52	130.8(3)
N22-C72-C62	120.6(3)
N22-C72-C82	116.6(3)
C62-C72-C82	122.7(3)
C72-C82-C92	111.9(2)
C102-C92-C82	112.6(2)
C92-C102-C112	113.4(2)
N22-C122-C132	103.5(3)
C142-C132-C122	105.7(3)
C152-C142-C132	104.1(3)
N22-C152-C142	103.3(3)
C23-S13-C53	91.03(15)
O13-N13-O23	122.3(3)
O13-N13-C23	120.2(3)
O23-N13-C23	117.6(3)
C73-N23-C123	123.3(2)
C73-N23-C153	125.9(2)
C123-N23-C153	110.7(2)
C33-C23-N13	126.4(3)
C33-C23-S13	113.1(2)
N13-C23-S13	120.5(2)
C23-C33-C43	111.5(3)
C33-C43-C53	115.0(3)
C43-C53-C63	123.0(3)
C43-C53-S13	109.3(2)
C63-C53-S13	127.8(2)
C73-C63-C53	130.6(3)
N23-C73-C63	121.0(3)
N23-C73-C83	116.3(3)
C63-C73-C83	122.7(3)
C73-C83-C93	112.1(2)
C103-C93-C83	112.1(2)
C113-C103-C93	113.1(3)
N23-C123-C133	103.4(3)
C123-C133-C143	103.8(3)
C153-C143-C133	102.7(3)
N23-C153-C143	103.6(2)