New insights into Chalcogen bonding provided by cocrystal structures of benzisoselenazolinone derivatives and nitrogen bases.

Thomas Fellowes,[1] Jonathan White[1,*]

1. School of Chemistry and the BIO-21 Institute, University of Melbourne

*Corresponding author: whitejm@unimelb.edu.au

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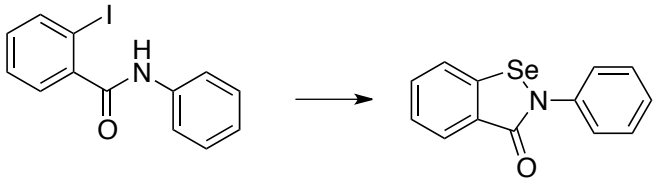
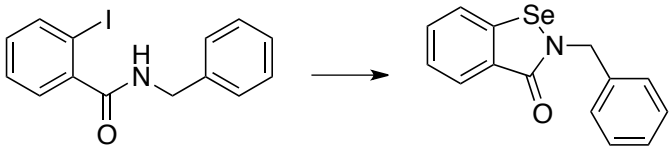
Synthetic Procedures

2-phenylbenzo[d][1,2]selenazol-3(2H)-one: **1a**



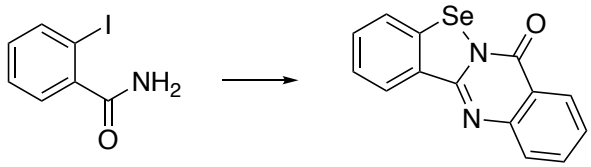
Copper iodide (98.4 mg, 0.517 mmol) and 1,10-phenanthroline (83.1 mg, 0.461 mmol) were stirred in anhydrous DMF (3 mL) for 15 mins at r.t., then 2-iodo-N-phenylbenzamide (653.2 mg, 2.021 mmol), selenium (196.9 mg, 2.495 mmol) and potassium carbonate (627.3 mg, 4.539 mmol) were added sequentially under a flow of argon. The mixture was heated at 110˚C for 8h, when TLC showed consumption of starting material. The mixture was then tipped into brine (30 mL) and stirred to form a brown precipitate, which was extracted into DCM (40 mL) and washed with water (2 x 20mL). The DCM solution was filtered through a silica plug, then evaporated, and the residue applied to a SNAP 25g silica cartridge, eluting with a petroleum ether/ethyl acetate gradient. The major peak was evaporated to afford colourless crystals of **1a** (378.8 mg, 69%, m.p. 179.1-180.3˚C, lit. mp 180-181).[1] ^{77}Se NMR δ 959.66

2-benzylbenzo[*d*][1,2]selenazol-3(2*H*)-one: **1b**



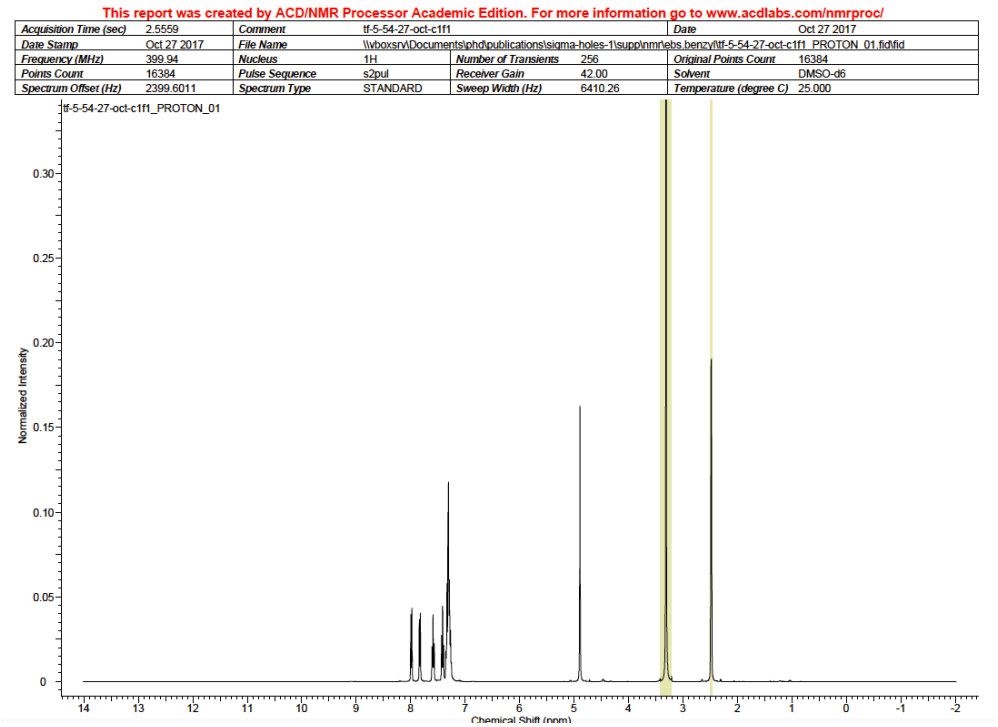
Copper iodide (95.8 mg, 0.503 mmol) and 1,10-phenanthroline (93.8 mg, 0.521 mmol) were stirred in anhydrous DMF (3 mL) for 15 mins at r.t., then N-benzyl-2-iodobenzamide (860.9 mg, 2.553 mmol), selenium (256.6 mg, 3.249 mmol) and potassium carbonate (542.2 mg, 3.923 mmol) were added sequentially under a flow of argon. The mixture was heated at 110˚C for 5h, when TLC showed consumption of starting material. The mixture was then tipped into brine (30 mL) and stirred to form a solid mass, which was dissolved in DCM (40 mL) and washed with water (2 x 20mL). The DCM solution was filtered through a silica plug, then evaporated, and the residue applied to a SNAP 50g silica cartridge, eluting with a petroleum ether/ethyl acetate gradient. The major peak was evaporated to afford pale yellow crystals of **1b** (396.4 mg, 53%, m.p. 137.8-138.8˚C). ^{77}Se NMR δ 884.02. Crystals suitable for x-ray analysis were obtained from dichloromethane/pentane.

5*H*-benzo[4,5][1,2]selenazolo[2,3-*a*]quinazolin-5-one: **3**

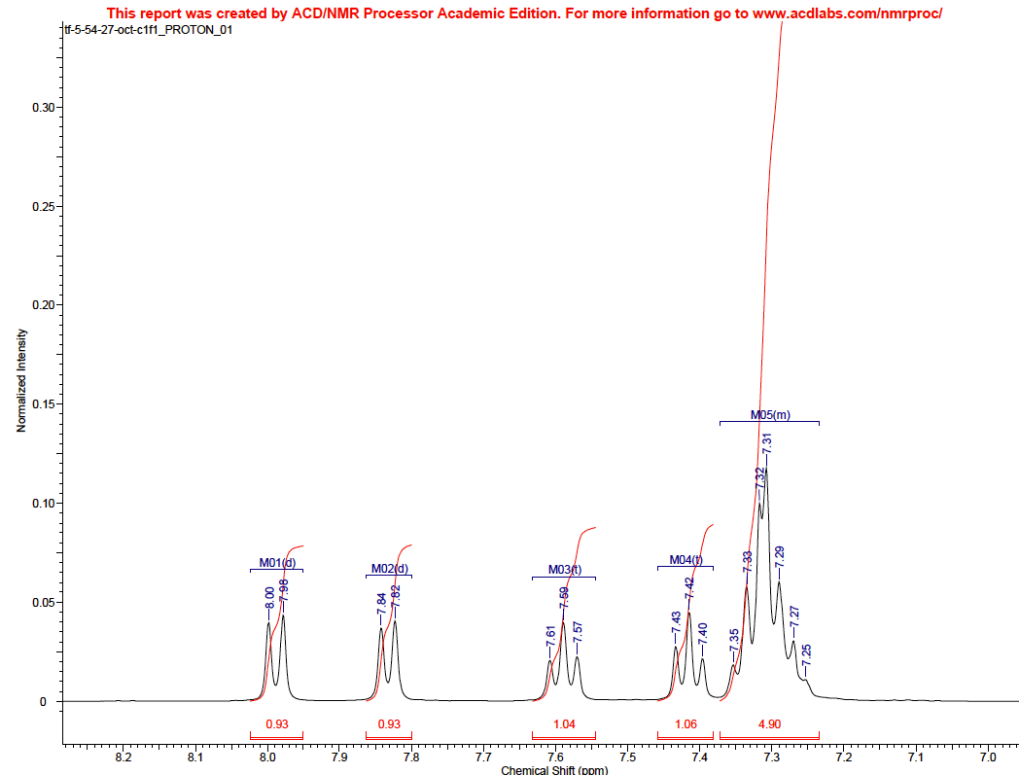


Copper iodide (96.4 mg, 0.503 mmol) and 1,10-phenanthroline (85.7 mg, 0.476 mmol) were stirred in anhydrous DMF (4 mL) for 10 mins at r.t., then 2-iodobenzamide (510.6 mg, 2.067 mmol), selenium (209.5 mg, 2.653 mmol) and potassium carbonate (506.3 mg, 3.663 mmol) were added sequentially under a flow of argon. The mixture was heated at 110˚C for 12h, when TLC showed consumption of starting material. The mixture was then tipped into brine (30 mL) and stirred to form a solid mass, which was extracted into ethyl acetate (20 mL) and washed with water (2 x 20mL). The DCM solution was filtered through a silica plug, then evaporated, and the residue applied to a SNAP 50g silica cartridge, eluting with a petroleum ether/ethyl acetate gradient. The major peak was evaporated to afford pale yellow crystals of **3** (45.8 mg,

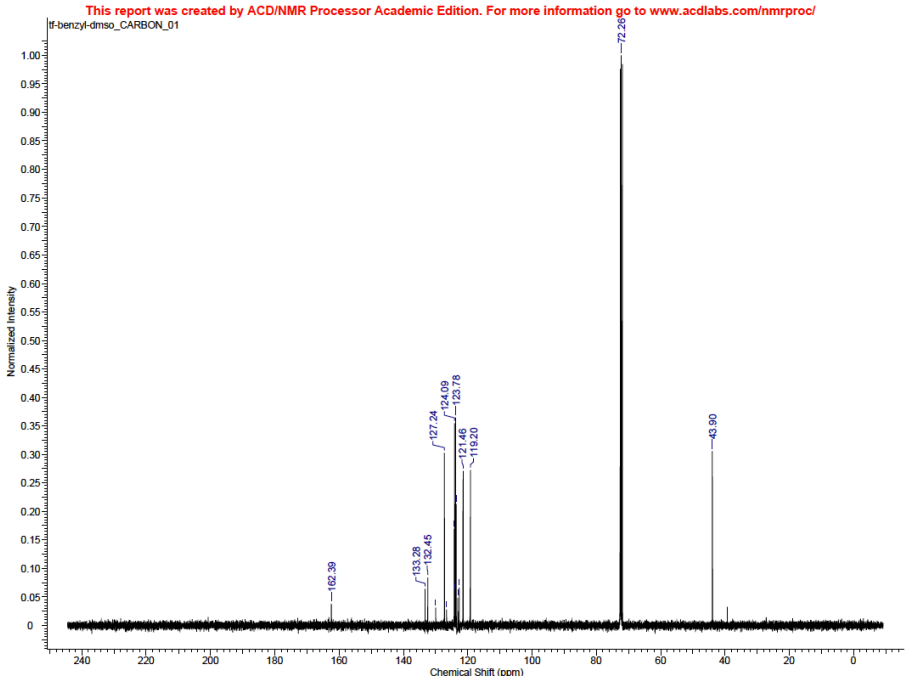
15%, m.p. 267-268˚C). ^{77}Se NMR δ 992.48. Crystals suitable for x-ray analysis were obtained from dichloromethane/pentane.



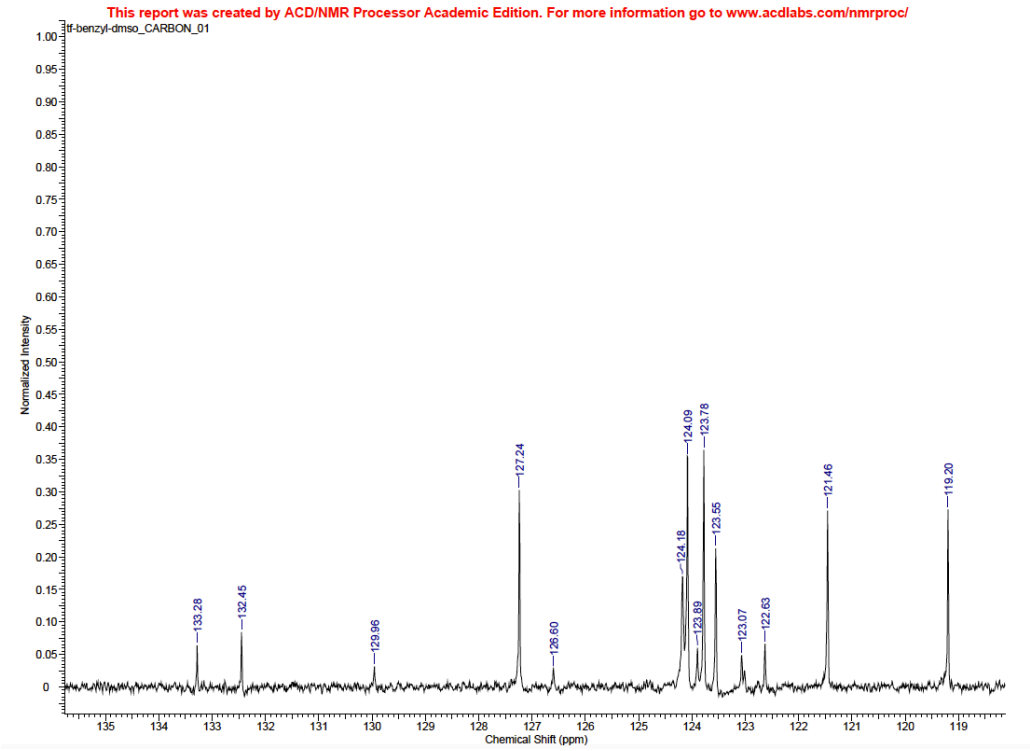
SUPP-Figure 1. ^{1}H nmr spectrum of **1b** in D6-DMSO



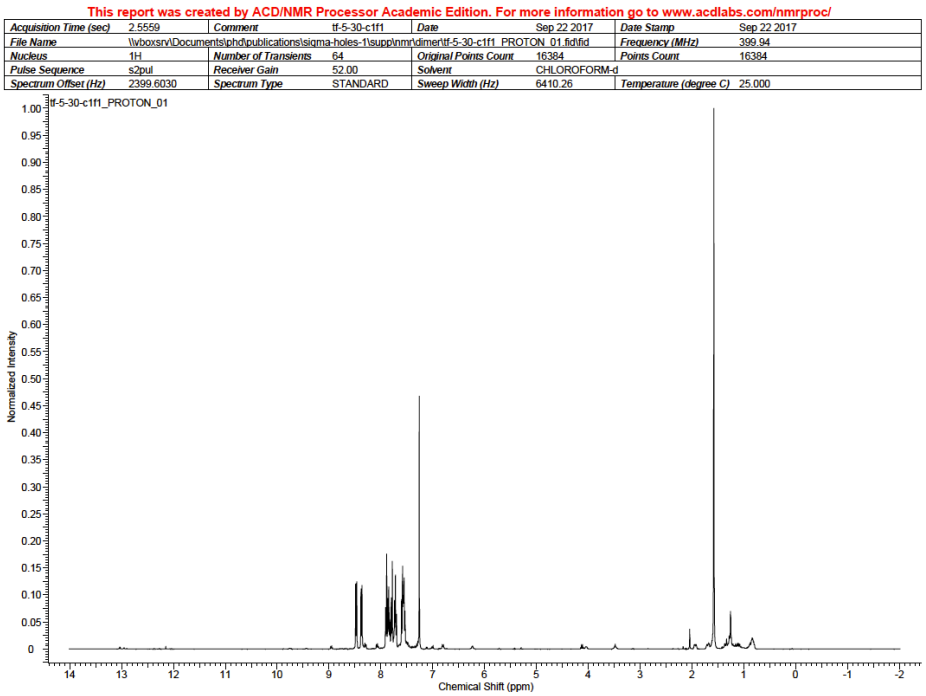
SUPP-Figure 2. ^{1}H nmr spectrum of **1b** in D6-DMSO, expanded aromatic region.



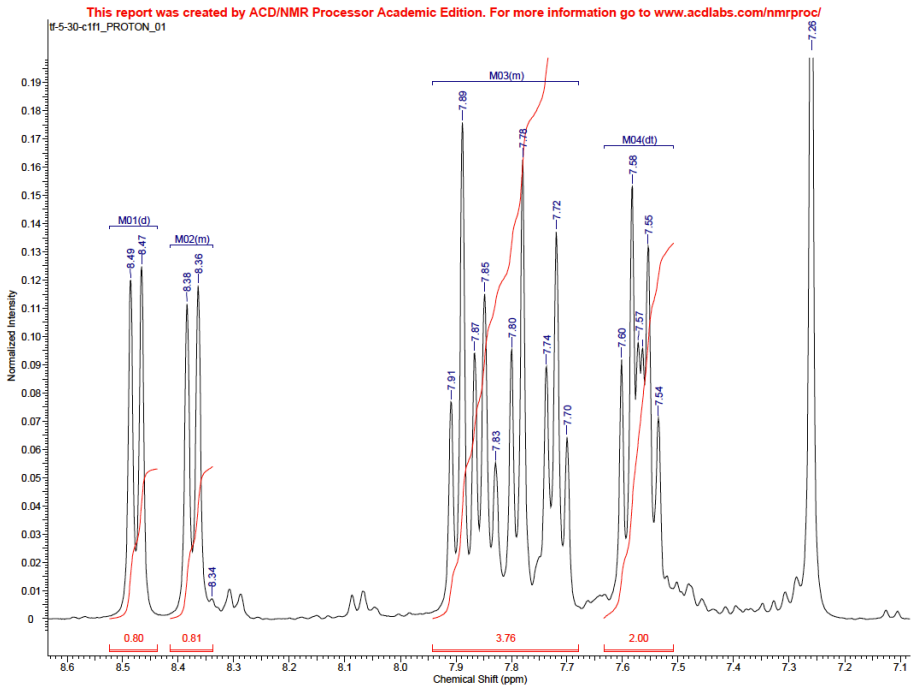
SUPP-Figure 3. ^{13}C nmr spectrum of **1b** in D6-DMSO.



SUPP-Figure 3. ^{13}C nmr spectrum of **1b** in D6-DMSO, expanded.



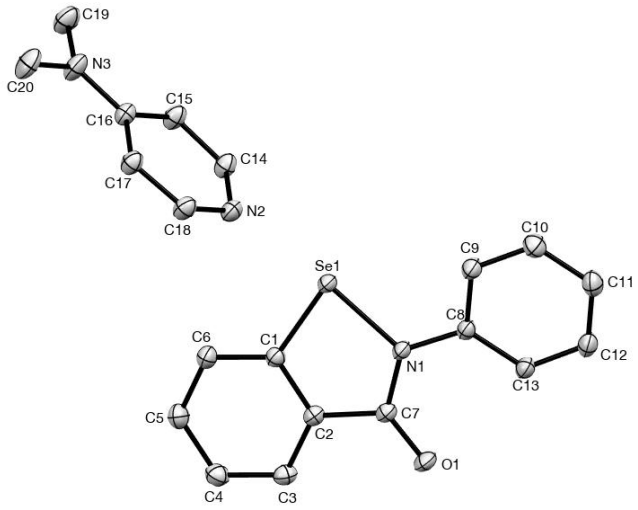
SUPP-Figure 5. ^{1}H nmr spectrum of **3** in CDCl3.



SUPP-Figure 6. ^{1}H nmr spectrum of **3** in CDCl3.

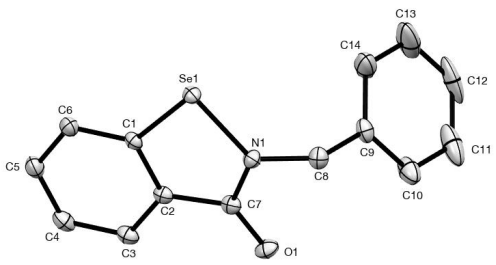
(1) Crystallography

Intensity data was collected on an Oxford Diffraction SuperNova CCD diffractometer using either Cu-Kα or Mo-Kα radiation at 130.0(1)K, or on a Rigaku XtalLAB Synergy at 100.0(1)K. Compound **1b**.DMAP.H_2O underwent a destructive phase change when cooling to 130 K, therefore data were collected at 200K. Data for **3** was collected on the MX1 beamline[2] at the Australian Synchrotron. The temperature was maintained using an Oxford Cryostream cooling device. The structures were solved by direct methods and difference Fourier synthesis.[3] Thermal ellipsoid plot was generated using the program ORTEP-3[4] integrated within the WINGX[5] suite of programs.



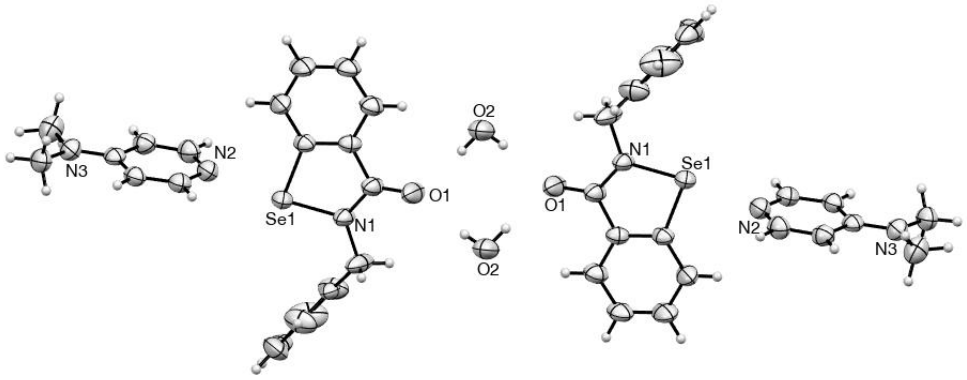
SUPP-Figure 7. Thermal ellipsoid plot for **1a**.DMAP. Ellipsoids are at the 30% probability level.

Crystal data for **1a**.DMAP. $C_{20}H_{19}N_3OSe$, *M* = 396.34, *T* = 130.0 K, λ = 0.71073 Å, Triclinic, space group P-1, *a* = 8.3674(3) *b* = 9.8399(5), *c* =10.6622(5) *Å*, α = 93.296(4)°, β = 93.021(4)° γ = 101.210(4)° *V* = 857.86(7) *Å*^{3}, Z = 2, D_c = 1.534 mg M^{-3} μ(Mo-Kα) 2.201 mm^{-1}, F(000) = 404 crystal size 0.52 x 0.34 x 0.23 mm^3, 11339 reflections measured θ_{max} = 36.66°, 7889 independent reflections [R(int) = 0.0163], the final R was 0.0293 [I > 2σ(I), 6882 data] and *w*R(F^2) was 0.0721 (all data), GOF 0.992. CCDC 1867205. From dichloromethane/pentane (70%) m.p. 111.3-112.1°C.



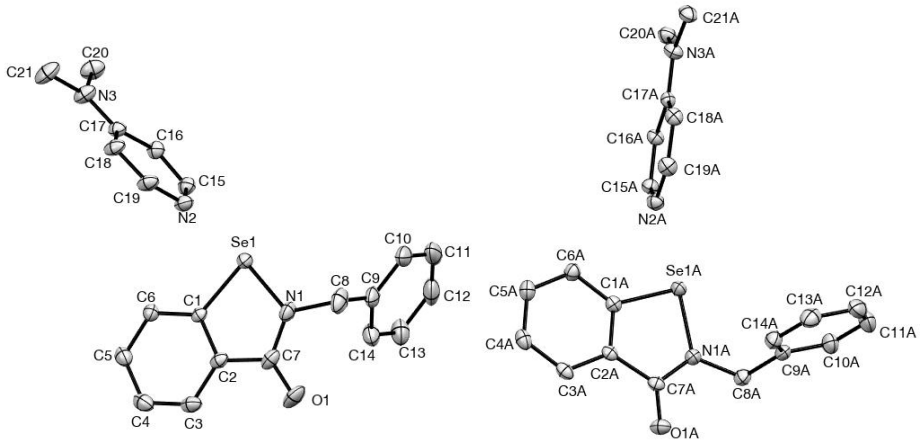
SUPP-Figure 8. Thermal ellipsoid plot of **1b**. Ellipsoids are at the 30% probability level.

Crystal data for **1b**. $C_{14}H_{11}NOSe$, M = 288.20, T = 100.0 K, λ = 0.71073 Å, Orthorhombic, space group $Pca2_1$, a = 11.7848(3), b = 4.5869(1), c =21.3572(5) Å, V = 1154.48(5) Å^3, Z = 4, D_c = 1.658 mg M^{-3} μ(Mo-Kα) 3.233 mm^{-1}, F(000) = 576 crystal size 0.63 x 0.54 x 0.22 mm^3, 44918 reflections measured θ_{max} = 45.38°, 9588 independent reflections [R(int) = 0.0481], the final R was 0.0331 [I > 2σ(I), 7848 data] and wR(F^2) was 0.0792 (all data), GOF 1.063. CCDC 1867211.



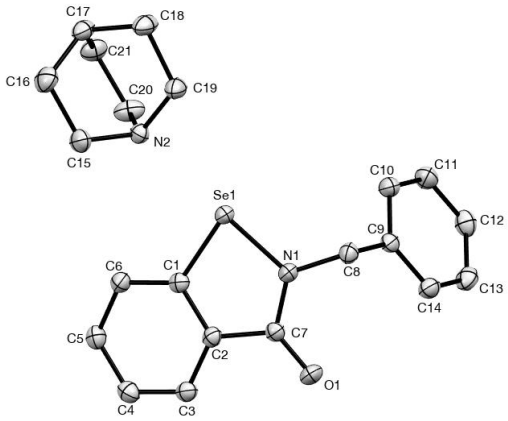
SUPP-Figure 9. Thermal ellipsoid plot for **1b.DMAP.H_2O**. Ellipsoids are at the 30% probability level.

Crystal data for **1b**.DMAP.H_2O. $C_{21}H_{21}N_3OSe.(H_2O)$, M = 428.38, T = 200.0 K, λ = 0.71073 Å, Triclinic, space group P-1, a = 9.6254(2), b = 10.2486(2), c =10.6505(2) Å, α = 83.660(2)°, β = 76.398(2)° γ = 78.423(2)° V = 998.19(4) Å^3, Z = 2, D_c = 125 mg M^{-3} μ(Mo-Kα) 1.901 mm^{-1}, F(000) = 440 crystal size 0.41 x 0.32 x 0.23 mm^3, 30047 reflections measured θ_{max} = 41.06°, 12528 independent reflections [R(int) = 0.0267], the final R was 0.0456 [I > 2σ(I), 6303 data] and wR(F^2) was 0.1219 (all data), GOF 1.000. CCDC 1867213. From THF in an open flask (90%) m.p. 96-97°C



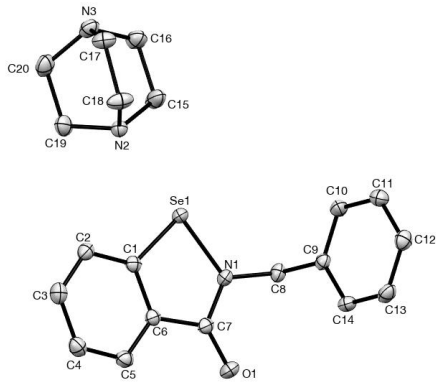
SUPP-Figure 10. Thermal ellipsoid plot for the two independent molecules **1b.**DMAP. Ellipsoids are at the 30% probability level.

Crystal data for **1b**.DMAP. $C_{21}H_{21}N_3OSe$, *M* = 410.37, *T* = 130.0 K, λ = 0.71073 Å, Triclinic, space group P-1, *a* = 9.6002(4), *b* = 10.2109(4), *c* =19.8380(7) *Å*, α = 78.710(3)°, β = 84.901(3)° γ = 77.458(4)° *V* = 1859.33(13) *Å*^{3}, Z = 4, Z' = 2 D_c = 1.466 mg M^{-3} μ(Mo-Kα) 2.034 mm^{-1}, F(000) = 840 crystal size 0.65 x 0.24 x 0.37 mm^3, 36541 reflections measured θ_{max} = 40.95°, 23437 independent reflections [R(int) = 0.0264], the final R was 0.0448 [I > 2σ(I), 15177 data] and *w*R(F^2) was 0.1120 (all data), GOF 1.044. CCDC 1867209. From dichloromethane/pentane (60%) m.p. 86.1-92.5°C.



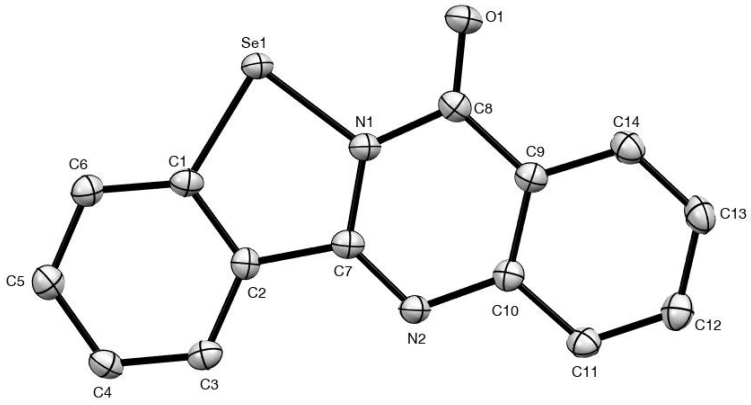
SUPP-Figure 11. Thermal ellipsoid plot for **1b**.QUINUCLIDINE. Ellipsoids are at the 30% probability level.

Crystal data for **1b**.QUINUCLIDINE. $C_{21}H_{24}N_2OSe$, *M* = 399.38, *T* = 130.0 K, λ = 1.54184 Å, Monoclinic, space group $P2_1/c$, *a* = 10.1610(2), *b* = 16.0506(3), *c* =11.4300(2) *Å*, β = 104.622(2)° *V* = 1803.75(6) *Å*^{3}, Z = 4, D_c = 1.471 mg M^{-3} μ(Cu-Kα) 3.895 mm^{-1}, F(000) = 824 crystal size 0.29 x 0.10 x 0.03 mm^3, 12588 reflections measured θ_{max} = 77.19°, 3771 independent reflections [R(int) = 0.0379], the final R was 0.0329 [I > 2σ(I), 3397 data] and *w*R(F^2) was 0.0849 (all data), GOF 1.028. CCDC 1867207. From chloroform pentane (50%) m.p. 135.2-137.4°C.



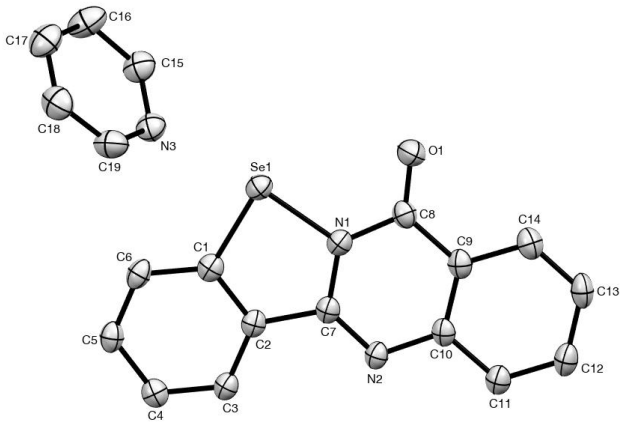
SUPP-Figure 12. Thermal ellipsoid plot for **1b**.DABCO. Ellipsoids are at the 30% probability level.

Crystal data for **1b**.DABCO. $C_{20}H_{23}N_3OSe$, M = 400.37, T = 130.0 K, λ = 1.54184 Å, Monoclinic, space group $P2_1/c$, a = 10.1249(2), b = 15.9246(3), c =11.4660(2) *Å*, β = 106.572(2)° V = 1771.93(6) *Å*^{3}, Z = 4, D_c = 1.501 mg M^{-3} μ(Cu-Kα) 2.965 mm^{-1}, F(000) = 824 crystal size 0.37 x 0.17 x 0.04 mm^3, 13121 reflections measured θ_{max} = 77.12°, 3711 independent reflections [R(int) = 0.0280], the final R was 0.0258 [I > 2σ(I), 3333 data] and *w*R(F^2) was 0.0657 (all data), GOF 1.056. CCDC 1867206. From dichloromethane/pentane (65%) m.p. 131.4-133.3°.C



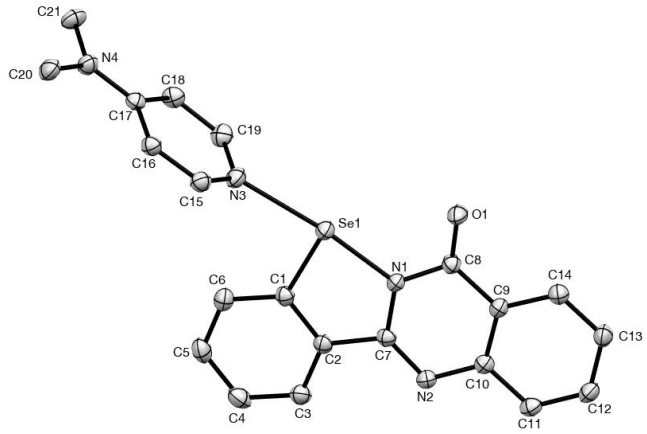
SUPP-Figure 13. Thermal ellipsoid plot of **3**. Ellipsoids are at the 30% probability level.

Crystal data for **3**. $C_{14}H_8N_2O$ Se, M = 299.18, T = 100.0 K, λ = 0.71092 Å, Orthorhombic, space group $Pca2_1$, a = 17.371(4), b = 5.3080(11), c =11.633(2) *Å*, V = 1072.6(4) *Å*^{3}, Z = 4, D_c = 1.853 mg M^{-3} 3.486 mm^{-1}, F(000) = 592 crystal size 0.15 x 0.10 x 0.02 mm^3, 16031 reflections measured θ_{max} = 31.56°, 2967 independent reflections [R(int) = 0.0363], the final R was 0.0271 [I > 2σ(I), 2061 data] and *w*R(F^2) was 0.0751 (all data), GOF 1.129. CCDC 1867208.



SUPP- 14. Thermal ellipsoid plot for **3**-PYR. Ellipsoids are at the 30% probability level.

Crystal data for **3**-PYR. $C_{19}H_{13}N_3OSe$, *M* = 378.28, *T* = 130.0 K, λ = 1.54184 Å, Monoclinic, space group $P2_1/c$, *a* = 20.7476(9), *b* = 4.9407(2), *c* =17.6687(7) *Å*, β = 107.376(4)° *V* = 1156.27(5) *Å*^{3}, Z = 4, D_c = 1.454 mg M^{-3} μ(CuKα) 3.018 mm^{-1}, F(000) = 760 crystal size 0.56 x 0.05 x 0.03 mm^3, 5766 reflections measured θ_{max} = 75.76°, 3419 independent reflections [R(int) = 0.0301], the final R was 0.0346 [I > 2σ(I), 2889 data] and *w*R(F^2) was 0.0955 (all data), GOF 1.054. CCDC 1867211. From dichloromethane/pentane (70%) m.p. 247.5-248.4°C.



SUPP-Figure 15. Thermal ellipsoid plot for **3**.DMAP. Ellipsoids are at the 30% probability level.

Crystal data for **3**.DMAP. $C_{21}H_{18}N_4OSe$, *M* = 421.35, *T* = 100.0 K, λ = 0.71073Å, Triclinic, space group P-1, *a* = 8.8093(2) *b* = 10.7445(2), *c* =10.9812(2) *Å*, α = 111.687(2)°, β = 109.283(2)° γ = 96.631(2)° *V* = 877.57(3) *Å*^{3}, Z = 2, D_c = 1.595 mg M^{-3} μ(Mo-Kα) 2.159 mm^{-1}, F(000) = 428 crystal size 0.18 x 0.11 x 0.06 mm^3, 56053 reflections measured θ_{max} = 41.07°, 11273 independent reflections [R(int) = 0.0547], the final R was 0.0358 [I > 2σ(I), 8667 data] and *w*R(F^2) was 0.0872 (all data), GOF 1.048. CCDC 1867212. From dichloromethane/pentane (80%) m.p. 248.8-249.4°C.

(1) Computational:

Structures were optimised at the wB97XD level of theory[6] using the def2TZVP basis set[7] as implemented in the Gaussian09 software package, and NBO calculations performed using the same[8,9]. Minima were verified by normal mode analysis. An ultrafine grid and tightened SCF convergence criteria were used for all calculations (`int(ultrafine)` and `scf(conver=12)`).

Structures obtained from our crystallographic studies were optimised first at the HF/6-31G(d,p) level of theory, then at ωB97XD/Def2TZVP using tight SCF convergence criteria and an ultrafine grid. Default geometric convergence criteria were used for all structures, except 1b.DMAP.H2O, where not all the displacement criteria would not converge. Using the optimised geometries, a frequency calculation was performed to verify the nature of the stationary point, and NBO analysis was performed using the NBOv3.1 software package[1].

1a

Sum of electronic and zero-point Energies= -3032.219044
Sum of electronic and thermal Energies= -3032.206520
Sum of electronic and thermal Enthalpies= -3032.205576
Sum of electronic and thermal Free Energies= -3032.260082

1	Se			
2	O	3.9263341		
3	N	1.8586549	21.2955737	
4	C	1.8828975	86.5878265	-0.8628750
5	C	1.3881097	127.4561030	-179.6763426
6	H	1.0823223	121.4057586	0.0558973
7	C	1.3861891	111.3046786	0.3557366
8	C	1.2116685	12.6716401	-178.9477884
9	C	1.3836164	118.1096321	-179.9487653
10	H	1.0827052	119.2295770	179.9460698
11	C	1.4167426	119.5966508	-179.8945224
12	C	1.3945426	121.1348840	-0.0942261
13	H	1.0819348	119.7352290	-179.9346331
14	C	1.3811323	120.1640003	0.0631690
15	H	1.0826388	122.0151557	-179.9364773
16	C	1.3902704	119.7163996	-42.6326667
17	H	1.0832734	119.8720860	-2.2442198
18	C	1.3909713	120.3931437	136.5063442
19	H	1.0794624	119.7485625	1.5304023
20	C	1.3841782	119.5614111	-179.4062520
21	H	1.0825031	119.2292200	-179.6396056
22	C	1.3853640	120.0575610	178.6109641
23	H	1.0824192	119.4925105	-179.8521963
24	C	1.3853012	120.2263769	0.8345981
25	H	1.0822405	120.2243031	179.5647760

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1b

Sum of electronic and zero-point Energies= -3071.508578
Sum of electronic and thermal Energies= -3071.494825

Sum of electronic and thermal Enthalpies= -3071.493881
Sum of electronic and thermal Free Energies= -3071.552123

1	C			
2	C	1.3884792		
3	C	1.3873599	120.1916504	
4	C	1.3880803	121.1701378	0.0647332
5	C	1.3836685	118.1460727	0.0476848
6	C	1.3813065	119.1910758	-0.1460157
7	H	1.0826735	121.9965886	-179.8917379
8	H	1.0823187	121.3759976	-179.9410190
9	H	1.0827222	119.2274557	179.9561670
10	H	1.0819618	120.1098567	-179.9119694
11	N	2.3353473	157.4509653	178.1377394
12	C	1.3710777	36.4901344	3.1505603
13	O	1.2159566	123.9196266	179.9724773
14	C	1.4498778	158.9822129	6.9674812
15	H	1.0911921	105.2957010	-16.6426178
16	H	1.0927417	109.3335904	-132.4498080
17	C	1.5087433	113.1000722	104.1532252
18	C	1.3873956	120.9984507	118.8463180
19	C	1.3920915	119.8331428	-60.7599814
20	C	1.3884690	120.5627134	-179.6530508
21	H	1.0844296	119.6383559	0.3364604
22	C	1.3835220	120.3726916	179.5303850
23	H	1.0840437	119.3179420	-0.6649507
24	C	1.3845340	119.9570058	0.1510732
25	H	1.0826777	119.8722809	179.9574888
26	H	1.0826925	119.8216103	179.8917885
27	H	1.0826103	120.1281765	179.8932455
28	Se	1.8488122	80.0485587	-179.5806233

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3

Sum of electronic and zero-point Energies= -3124.499546
Sum of electronic and thermal Energies= -3124.486722
Sum of electronic and thermal Enthalpies= -3124.485778
Sum of electronic and thermal Free Energies= -3124.539686

1	Se			
2	C	4.0812705		
3	H	1.0821357	132.4447083	
4	N	1.8540841	63.8120142	0.0010670
5	C	1.3899622	13.4854202	0.0007223
6	C	1.3804554	105.6591521	-179.9992538
7	H	1.0818234	119.9829021	-180.0000000
8	C	1.3849557	118.7418440	179.9921968
9	C	1.3929037	120.2982493	0.0004654
10	C	2.4737014	141.6985423	179.9488400
11	H	1.0820881	87.6780212	-179.9503810

12	N	2.3482535	143.8939060	-0.0058541
13	O	1.2142675	120.0527450	0.0583169
14	C	2.3994033	120.2767417	0.0558484
15	H	1.0829541	149.3455080	179.9945437
16	C	1.3880549	120.7539384	-0.0009832
17	H	1.0822723	121.2018840	-179.9993641
18	C	1.3781821	87.8789198	-179.9828745
19	C	1.2864454	29.0701608	0.0072699
20	C	1.3734620	150.7126981	0.0639121
21	H	1.0819537	120.2327647	179.9855759
22	C	1.3835260	118.4659654	0.0008173
23	H	1.0825491	119.2527058	179.9996221
24	C	1.3735894	91.0750197	-0.0081821
25	H	1.0818262	121.5706056	-179.9967501
26	C	1.3981798	30.7208789	0.0448287

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DABCO

Sum of electronic and zero-point Energies= -345.165427
Sum of electronic and thermal Energies= -345.159195
Sum of electronic and thermal Enthalpies= -345.158251
Sum of electronic and thermal Free Energies= -345.195837

1	C			
2	C	1.5555449		
3	H	1.0921801	111.4299206	
4	H	1.0921795	111.4214717	-119.9859436
5	H	1.0921419	111.4262578	-119.9893689
6	H	1.0921883	111.4172852	-0.0054857
7	C	2.3802033	89.9983354	90.0122144
8	H	1.0921795	143.7245112	128.0594586
9	H	1.0921768	90.0316288	-111.4618732
10	C	1.5555097	89.9808272	-0.0312566
11	H	1.0921877	111.4217196	150.0654211
12	H	1.0921419	111.4261838	-89.9472765
13	C	2.3795877	90.0009877	-59.9799549
14	H	1.0921972	143.7818479	128.1036478
15	H	1.0921933	90.0671189	-111.4137619
16	C	1.5552150	90.0171963	-0.0290311
17	H	1.0921879	111.4319515	150.0287056
18	H	1.0921866	111.4343045	-89.9798879
19	N	1.4612966	109.8803169	-29.9810800
20	N	1.4601944	35.4712750	125.8737955

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Quinuclidine

Sum of electronic and zero-point Energies= -329.134608
Sum of electronic and thermal Energies= -329.128070
Sum of electronic and thermal Enthalpies= -329.127126

Sum of electronic and thermal Free Energies= -329.164686

1	C			
2	C	2.4942004		
3	C	1.5319785	36.3386500	
4	H	1.0917212	110.9547387	-120.5417920
5	H	1.0917212	110.9547387	120.5417920
6	H	1.0924203	109.9029278	-121.1968980
7	H	1.0924203	109.9029278	121.1968980
8	C	2.3841841	91.9673420	-30.0195110
9	H	1.0917207	143.1805291	130.0149574
10	H	1.0917211	89.7839708	-110.9598921
11	C	1.5319780	88.3699722	-125.5833112
12	H	1.0924204	109.9029537	-149.7608361
13	H	1.0924207	109.9029219	92.6329690
14	H	1.0905470	146.5036485	0.0000000
15	C	1.5319780	88.3699722	125.5833112
16	H	1.0924204	109.9029537	149.7608361
17	H	1.0924207	109.9029219	-92.6329690
18	C	1.5530757	107.8932021	28.5639209
19	H	1.0917207	110.9547691	120.5417741
20	H	1.0917211	110.9547593	-120.5417374
21	N	1.4590888	111.6406777	0.0000000

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pyridine

Sum of electronic and zero-point Energies= -248.193946
Sum of electronic and thermal Energies= -248.189710
Sum of electronic and thermal Enthalpies= -248.188766
Sum of electronic and thermal Free Energies= -248.220660

1	C			
2	C	2.2704500		
3	C	1.3869122	92.2781587	
4	C	1.3846956	118.4443388	0.0000000
5	C	1.3846956	118.5550049	0.0000000
6	H	1.0853905	120.2389374	180.0000000
7	H	1.0853905	147.4829039	180.0000000
8	H	1.0819265	120.2354201	180.0000000
9	H	1.0829780	120.7224975	180.0000000
10	H	1.0819265	121.3202411	180.0000000
11	N	1.3289769	31.3274584	180.0000000

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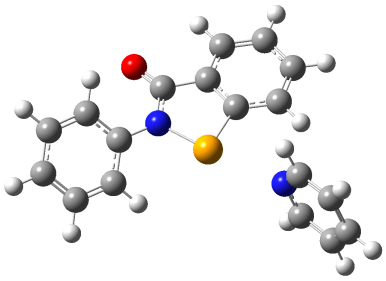
DMAP

Sum of electronic and zero-point Energies= -382.102731
Sum of electronic and thermal Energies= -382.094169
Sum of electronic and thermal Enthalpies= -382.093224
Sum of electronic and thermal Free Energies= -382.136857

1	C			
2	C	1.3808026		
3	C	1.4046426	119.3559934	
4	C	1.4046426	115.8748778	0.3767901
5	C	1.3808026	119.3559934	-0.3767901
6	N	1.3300770	124.9302183	0.1548689
7	H	1.0859224	116.0346500	179.8300493
8	H	1.0798793	119.0283866	179.7943145
9	H	1.0798793	121.6155999	179.5710330
10	H	1.0859224	119.0350782	-179.9323831
11	N	1.3652352	122.0625564	-179.5885966
12	C	1.4437309	119.9057191	-3.3849828
13	H	1.0957907	112.0576133	-60.8670174
14	H	1.0939866	111.4702318	60.4399707
15	H	1.0872508	109.2621481	179.4103638
16	C	1.4437309	119.9057191	-176.6517658
17	H	1.0872507	109.2621512	-179.4104195
18	H	1.0939866	111.4702318	-60.4399707
19	H	1.0957907	112.0576133	60.8670174

1a.pyridine



Sum of electronic and zero-point Energies= -3280.424880
Sum of electronic and thermal Energies= -3280.406071
Sum of electronic and thermal Enthalpies= -3280.405126
Sum of electronic and thermal Free Energies= -3280.477861

1	Se			
2	O	3.9551727		
3	N	1.8819337	21.0604606	
4	C	1.8913099	85.7488412	-1.1668389
5	C	1.3895733	127.9538230	-179.6368626
6	H	1.0798585	120.8148267	-0.1197066
7	C	1.3882780	111.5051745	0.3448728
8	C	1.2149392	12.0972319	-178.2111474
9	C	1.3837626	118.5024652	179.9682375
10	H	1.0830432	119.1022903	179.9386388
11	C	1.4129786	119.2992753	-179.1417793
12	C	1.3936862	121.2511494	-0.0740989
13	H	1.0821257	119.9211498	-179.9436410
14	C	1.3806286	119.8536010	0.0712306
15	H	1.0827126	122.0779540	-179.9774492
16	C	1.3926316	120.8617636	138.8408193
17	H	1.0791924	119.6337100	2.0189405
18	C	1.3917781	119.6313154	-39.9625213

19	H	1.0830340	119.7488008	-2.6500954
20	C	1.3853918	120.2733766	178.2630119
21	H	1.0826761	119.4559940	-179.9120670
22	C	1.3840847	119.7351919	-178.9590771
23	H	1.0827430	119.1699945	-179.6814353
24	C	1.3851516	120.2890245	0.7694628
25	H	1.0823495	120.3107241	179.5724280
26	N	2.7747786	176.1862272	11.9427787
27	C	1.3295429	118.8557489	87.5550336
28	C	1.3296664	120.6500075	-109.4961739
29	C	1.3851635	122.9385348	163.5034645
30	H	1.0846405	116.0526372	-16.3987233
31	C	1.3849906	122.9544827	-163.1836103
32	H	1.0847100	116.0573191	16.7777113
33	C	1.3849837	118.4821337	-0.0882708
34	H	1.0814967	120.1714230	179.9992543
35	H	1.0815144	120.1866838	179.9942150
36	H	1.0826250	120.5810362	-179.9499932

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
1. BD (1)Se 1 - N 3	/555. RY*(1) N 26	0.64	1.86	0.031
2. BD (1)Se 1 - C 4	/555. RY*(1) N 26	0.23	1.84	0.018
7. BD (1) C 4 - C 5	/555. RY*(1) N 26	0.05	1.97	0.009
7. BD (1) C 4 - C 5	/558. RY*(4) N 26	0.08	1.65	0.010
10. BD (1) C 5 - H 6	/771. BD*(2) N 26 - C 27	0.22	0.64	0.012
84. LP (1)Se 1	/555. RY*(1) N 26	0.10	1.94	0.013
84. LP (1)Se 1	/770. BD*(1) N 26 - C 27	0.42	1.38	0.021
84. LP (1)Se 1	/771. BD*(2) N 26 - C 27	0.24	0.82	0.014
84. LP (1)Se 1	/772. BD*(1) N 26 - C 28	0.48	1.38	0.023
85. LP (2)Se 1	/770. BD*(1) N 26 - C 27	0.16	0.89	0.011
85. LP (2)Se 1	/772. BD*(1) N 26 - C 28	0.17	0.89	0.011
85. LP (2)Se 1	/773. BD*(1) C 27 - C 29	0.10	0.90	0.009
85. LP (2)Se 1	/775. BD*(1) C 28 - C 31	0.09	0.90	0.008
from unit 2 to unit 1				
35. BD (1) N 26 - C 27	/736. BD*(1)Se 1 - N 3	0.16	1.11	0.012
36. BD (2) N 26 - C 27	/225. RY*(2) H 6	0.05	2.84	0.012
36. BD (2) N 26 - C 27	/736. BD*(1)Se 1 - N 3	0.16	0.54	0.009
36. BD (2) N 26 - C 27	/745. BD*(1) C 5 - H 6	0.16	0.88	0.011
37. BD (1) N 26 - C 28	/736. BD*(1)Se 1 - N 3	0.16	1.11	0.012
38. BD (1) C 27 - C 29	/736. BD*(1)Se 1 - N 3	0.14	0.98	0.011
39. BD (1) C 27 - H 30	/ 95. RY*(6)Se 1	0.05	1.88	0.009
40. BD (1) C 28 - C 31	/736. BD*(1)Se 1 - N 3	0.14	0.98	0.011
78. CR (1) N 26	/736. BD*(1)Se 1 - N 3	0.07	14.41	0.028
89. LP (1) N 26	/ 91. RY*(2)Se 1	0.81	1.71	0.034
89. LP (1) N 26	/ 97. RY*(8)Se 1	0.10	1.81	0.012
89. LP (1) N 26	/202. RY*(5) C 5	0.06	2.23	0.011
89. LP (1) N 26	/225. RY*(2) H 6	0.05	2.90	0.011
89. LP (1) N 26	/736. BD*(1)Se 1 - N 3	11.24	0.61	0.075
89. LP (1) N 26	/737. BD*(1)Se 1 - C 4	0.58	0.67	0.018
89. LP (1) N 26	/743. BD*(1) C 4 - C 7	0.28	1.07	0.016
89. LP (1) N 26	/745. BD*(1) C 5 - H 6	0.28	0.95	0.015
89. LP (1) N 26	/746. BD*(1) C 5 - C 9	0.23	1.10	0.014
771. BD*(2) N 26 - C 27	/736. BD*(1)Se 1 - N 3	0.19	0.13	0.009

771. BD*(2) N 26 - C 27	/745. BD*(1) C 5 - H 6	0.09	0.47	0.013
776. BD*(2) C 28 - C 31	/747. BD*(2) C 5 - C 9	0.06	0.03	0.002

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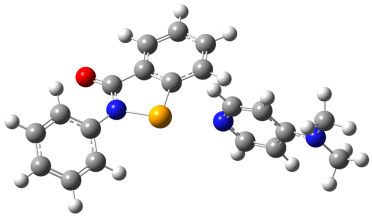
1a.DMAP



Sum of electronic and zero-point Energies= -3414.336379
Sum of electronic and thermal Energies= -3414.313262
Sum of electronic and thermal Enthalpies= -3414.312317
Sum of electronic and thermal Free Energies= -3414.394941

1	Se			
2	O	3.9659805		
3	N	1.8915810	20.9833163	
4	C	1.8930170	85.4265963	-1.4321749
5	C	1.3899136	127.9291698	-179.5438729
6	H	1.0796118	120.6891338	-0.0975812
7	C	1.3887834	111.6832305	0.4351984
8	C	1.2160983	11.9206376	-177.7073727
9	C	1.3837447	118.6013184	179.9759402
10	H	1.0831369	119.0751469	179.9479347
11	C	1.4116775	119.2727390	-179.0436119
12	C	1.3935689	121.2662159	-0.0715445
13	H	1.0822139	119.9646430	-179.9437657
14	C	1.3805573	119.7853604	0.0629848
15	H	1.0827429	122.0943925	-179.9716527
16	C	1.3931277	120.9816801	138.9038776
17	H	1.0791992	119.5881381	2.0603959
18	C	1.3922117	119.6145250	-39.8427276
19	H	1.0829431	119.7018555	-2.6675850
20	C	1.3854105	120.3214057	178.2300217
21	H	1.0827598	119.4450435	-179.9366060
22	C	1.3840461	119.7963240	-178.8959441
23	H	1.0828244	119.1643861	-179.6899829
24	C	1.3851797	120.3121649	0.7442392
25	H	1.0824050	120.3304663	179.5640581
26	N	2.6852413	175.6217105	11.2755927
27	C	1.3316321	120.0666523	86.0963373
28	C	1.3315949	121.6308369	-109.2712046
29	C	1.3769907	124.2186326	165.6331767
30	H	1.0850667	115.9290139	-14.3204883
31	C	1.3770286	124.2370210	-165.3755868
32	H	1.0851237	115.9423342	14.6399495
33	C	1.4072881	119.4631558	-0.1101593
34	H	1.0793761	118.9138594	-179.9619088
35	H	1.0793592	118.8964587	179.9447537
36	N	1.3591764	121.9735757	179.9799206
37	C	1.4457995	120.0444776	0.6013427
38	H	1.0944349	111.7086568	60.7127023
39	H	1.0867749	109.2298868	-179.9250372
40	H	1.0941991	111.6222919	-60.6788541
41	C	1.4457533	120.0634469	179.4880279

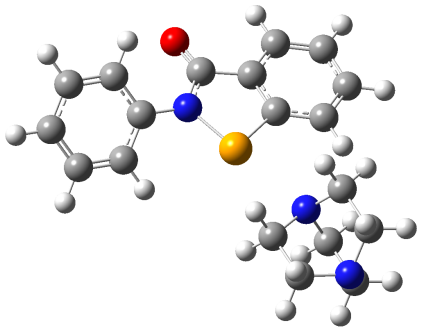
42	H	1.0941836	111.6111074	60.4380835
43	H	1.0867720	109.2309146	179.6679844
44	H	1.0944827	111.7280469	-60.9560407

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
1. BD (1)Se 1 - N 3	/568. RY*(1) N 26	0.78	1.85	0.034
1. BD (1)Se 1 - N 3	/570. RY*(3) N 26	0.09	1.47	0.010
2. BD (1)Se 1 - C 4	/568. RY*(1) N 26	0.29	1.83	0.021
2. BD (1)Se 1 - C 4	/887. BD*(1) N 26 - C 28	0.05	1.27	0.007
7. BD (1) C 4 - C 5	/568. RY*(1) N 26	0.06	1.97	0.009
7. BD (1) C 4 - C 5	/570. RY*(3) N 26	0.07	1.60	0.010
10. BD (1) C 5 - H 6	/100. LP (2) N 26	0.51	0.37	0.020
58. CR (3)Se 1	/886. BD*(1) N 26 - C 27	0.06	11.37	0.024
58. CR (3)Se 1	/887. BD*(1) N 26 - C 28	0.07	11.37	0.025
94. LP (1)Se 1	/100. LP (2) N 26	0.36	0.56	0.021
94. LP (1)Se 1	/568. RY*(1) N 26	0.13	1.94	0.014
94. LP (1)Se 1	/886. BD*(1) N 26 - C 27	0.57	1.38	0.025
94. LP (1)Se 1	/887. BD*(1) N 26 - C 28	0.62	1.38	0.026
94. LP (1)Se 1	/890. BD*(1) C 27 - H 30	0.05	1.25	0.007
94. LP (1)Se 1	/893. BD*(1) C 28 - H 32	0.05	1.25	0.007
95. LP (2)Se 1	/886. BD*(1) N 26 - C 27	0.23	0.89	0.013
95. LP (2)Se 1	/887. BD*(1) N 26 - C 28	0.24	0.89	0.013
95. LP (2)Se 1	/888. BD*(1) C 27 - C 29	0.12	0.92	0.010
95. LP (2)Se 1	/891. BD*(1) C 28 - C 31	0.11	0.92	0.009
from unit 2 to unit 1				
35. BD (1) N 26 - C 27	/852. BD*(1)Se 1 - N 3	0.24	1.09	0.015
36. BD (1) N 26 - C 28	/852. BD*(1)Se 1 - N 3	0.23	1.09	0.014
37. BD (1) C 27 - C 29	/852. BD*(1)Se 1 - N 3	0.17	0.98	0.012
40. BD (1) C 28 - C 31	/852. BD*(1)Se 1 - N 3	0.17	0.98	0.012
85. CR (1) N 26	/852. BD*(1)Se 1 - N 3	0.11	14.39	0.036
99. LP (1) N 26	/103. RY*(1)Se 1	0.19	1.33	0.015
99. LP (1) N 26	/104. RY*(2)Se 1	0.99	1.65	0.037
99. LP (1) N 26	/110. RY*(8)Se 1	0.11	1.78	0.013
99. LP (1) N 26	/118. RY*(16)Se 1	0.06	2.50	0.011
99. LP (1) N 26	/215. RY*(5) C 5	0.09	2.23	0.013
99. LP (1) N 26	/237. RY*(1) H 6	0.06	1.29	0.008
99. LP (1) N 26	/238. RY*(2) H 6	0.06	2.91	0.012
99. LP (1) N 26	/852. BD*(1)Se 1 - N 3	15.45	0.60	0.087
99. LP (1) N 26	/853. BD*(1)Se 1 - C 4	0.89	0.66	0.022
99. LP (1) N 26	/859. BD*(1) C 4 - C 7	0.35	1.06	0.018
99. LP (1) N 26	/861. BD*(1) C 5 - H 6	0.25	0.95	0.014
99. LP (1) N 26	/862. BD*(1) C 5 - C 9	0.25	1.09	0.015
100. LP (2) N 26	/852. BD*(1)Se 1 - N 3	0.40	0.39	0.013
100. LP (2) N 26	/861. BD*(1) C 5 - H 6	0.39	0.73	0.019
100. LP (2) N 26	/862. BD*(1) C 5 - C 9	0.09	0.87	0.010
889. BD*(2) C 27 - C 29	/863. BD*(2) C 5 - C 9	0.11	0.02	0.002
892. BD*(2) C 28 - C 31	/863. BD*(2) C 5 - C 9	0.11	0.02	0.002

1a.DABCO



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Sum of electronic and thermal Energies= -3377.377456
Sum of electronic and thermal Enthalpies= -3377.376512
Sum of electronic and thermal Free Energies= -3377.451475

1	Se			
2	O	3.9564238		
3	N	1.8827484	21.0268868	
4	C	1.8876172	85.6374986	-1.9172826
5	C	1.3883521	127.7038640	-179.2318203
6	H	1.0790971	120.8647744	0.1164292
7	C	1.3878659	111.7576556	0.6846769
8	C	1.2146229	12.1093275	-176.8719389
9	C	1.3834638	118.6508049	-179.9758275
10	H	1.0829773	119.2298227	179.9598326
11	C	1.4129875	119.1839545	-179.1132064
12	C	1.3936829	121.0987590	-0.1114112
13	H	1.0820431	119.8889934	-179.9271627
14	C	1.3809481	119.8962159	0.0148691
15	H	1.0827041	122.0377607	-179.8812354
16	C	1.3923305	120.8537892	137.3117000
17	H	1.0793244	119.6424615	1.9869163
18	C	1.3917125	119.5989823	-41.4826781
19	H	1.0830547	119.7089145	-2.7824551
20	C	1.3854778	120.2546974	178.2419924
21	H	1.0826802	119.4884544	-179.9784184
22	C	1.3841390	119.7271720	-178.9504145
23	H	1.0826922	119.1932912	-179.6586237
24	C	1.3852327	120.2676530	0.7751499
25	H	1.0823229	120.2937644	179.5385258
26	C	3.2317606	151.5591895	175.4654468
27	C	2.3847340	81.0668739	-146.3940480
28	C	2.3843851	81.7323015	152.5833573
29	C	1.5526672	169.8942713	-171.3187599
30	H	1.0917836	72.8112667	-53.5921468
31	H	1.0920262	74.4235800	60.7370475
32	H	1.0913643	144.1797106	-46.7518749
33	H	1.0912708	89.5178543	73.0345059
34	C	1.5544187	89.9700282	-175.0579347
35	C	1.5543871	89.6533779	174.4964083
36	H	1.0913871	144.2012297	46.9325482
37	H	1.0913301	89.9577322	-73.5877917

38	H	1.0914330	111.1883736	114.0694135
39	H	1.0914658	111.2245067	-126.1845480
40	H	1.0915645	111.2018495	149.5092463
41	H	1.0914525	111.2062076	-90.7575661
42	H	1.0915519	111.1906186	-150.5534244
43	H	1.0914944	111.2139964	89.7178781
44	N	1.4660130	35.6370257	48.5661257
45	N	1.4596046	109.9951503	-6.0190797

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
1. BD (1)Se 1 - N 3	/781. RY*(1) N 44	0.69	1.73	0.031
1. BD (1)Se 1 - N 3	/783. RY*(3) N 44	0.06	2.36	0.011
2. BD (1)Se 1 - C 4	/781. RY*(1) N 44	0.25	1.72	0.019
10. BD (1) C 5 - H 6	/870. BD*(1) C 26 - N 44	0.13	1.02	0.010
10. BD (1) C 5 - H 6	/871. BD*(1) C 27 - H 32	0.08	1.06	0.008
10. BD (1) C 5 - H 6	/873. BD*(1) C 27 - C 34	0.06	1.01	0.007
10. BD (1) C 5 - H 6	/875. BD*(1) C 28 - C 35	0.06	1.01	0.007
10. BD (1) C 5 - H 6	/876. BD*(1) C 28 - H 36	0.09	1.05	0.009
93. LP (1)Se 1	/781. RY*(1) N 44	0.06	1.82	0.009
93. LP (1)Se 1	/867. BD*(1) C 26 - C 29	0.79	1.18	0.028
93. LP (1)Se 1	/874. BD*(1) C 27 - N 44	0.45	1.19	0.021
93. LP (1)Se 1	/878. BD*(1) C 28 - N 44	0.48	1.19	0.021
94. LP (2)Se 1	/868. BD*(1) C 26 - H 30	0.08	0.75	0.007
94. LP (2)Se 1	/869. BD*(1) C 26 - H 31	0.06	0.74	0.006
94. LP (2)Se 1	/873. BD*(1) C 27 - C 34	0.10	0.69	0.008
94. LP (2)Se 1	/874. BD*(1) C 27 - N 44	0.15	0.71	0.009
94. LP (2)Se 1	/875. BD*(1) C 28 - C 35	0.10	0.69	0.007
94. LP (2)Se 1	/878. BD*(1) C 28 - N 44	0.17	0.71	0.010
from unit 2 to unit 1				
36. BD (1) C 26 - H 30	/100. RY*(1)Se 1	0.08	1.39	0.009
36. BD (1) C 26 - H 30	/103. RY*(4)Se 1	0.13	1.74	0.013
36. BD (1) C 26 - H 30	/833. BD*(1)Se 1 - N 3	0.08	0.75	0.007
36. BD (1) C 26 - H 30	/834. BD*(1)Se 1 - C 4	0.11	0.80	0.008
37. BD (1) C 26 - H 31	/103. RY*(4)Se 1	0.12	1.74	0.013
37. BD (1) C 26 - H 31	/833. BD*(1)Se 1 - N 3	0.08	0.75	0.007
37. BD (1) C 26 - H 31	/834. BD*(1)Se 1 - C 4	0.09	0.80	0.008
38. BD (1) C 26 - N 44	/833. BD*(1)Se 1 - N 3	0.15	0.95	0.011
39. BD (1) C 27 - H 32	/234. RY*(1) H 6	0.20	1.57	0.016
39. BD (1) C 27 - H 32	/842. BD*(1) C 5 - H 6	0.25	1.09	0.015
40. BD (1) C 27 - H 33	/104. RY*(5)Se 1	0.08	1.58	0.010
40. BD (1) C 27 - H 33	/105. RY*(6)Se 1	0.06	2.12	0.010
40. BD (1) C 27 - H 33	/106. RY*(7)Se 1	0.07	2.02	0.011
41. BD (1) C 27 - C 34	/833. BD*(1)Se 1 - N 3	0.10	0.84	0.008
42. BD (1) C 27 - N 44	/833. BD*(1)Se 1 - N 3	0.08	0.95	0.008
42. BD (1) C 27 - N 44	/842. BD*(1) C 5 - H 6	0.05	1.29	0.007
43. BD (1) C 28 - C 35	/833. BD*(1)Se 1 - N 3	0.10	0.84	0.008
44. BD (1) C 28 - H 36	/234. RY*(1) H 6	0.25	1.57	0.018
44. BD (1) C 28 - H 36	/842. BD*(1) C 5 - H 6	0.33	1.09	0.017
45. BD (1) C 28 - H 37	/104. RY*(5)Se 1	0.06	1.58	0.009
45. BD (1) C 28 - H 37	/105. RY*(6)Se 1	0.07	2.12	0.011
45. BD (1) C 28 - H 37	/108. RY*(9)Se 1	0.06	2.35	0.011
46. BD (1) C 28 - N 44	/833. BD*(1)Se 1 - N 3	0.08	0.95	0.008
46. BD (1) C 28 - N 44	/842. BD*(1) C 5 - H 6	0.06	1.29	0.008

91. CR (1) N 44	/833. BD*(1)Se 1 - N 3	0.06	14.43	0.026
98. LP (1) N 44	/100. RY*(1)Se 1	0.08	1.19	0.009
98. LP (1) N 44	/101. RY*(2)Se 1	0.99	1.47	0.035
98. LP (1) N 44	/103. RY*(4)Se 1	0.06	1.55	0.009
98. LP (1) N 44	/104. RY*(5)Se 1	0.05	1.38	0.008
98. LP (1) N 44	/106. RY*(7)Se 1	0.07	1.82	0.010
98. LP (1) N 44	/110. RY*(11)Se 1	0.07	1.70	0.010
98. LP (1) N 44	/115. RY*(16)Se 1	0.07	2.73	0.013
98. LP (1) N 44	/833. BD*(1)Se 1 - N 3	9.58	0.55	0.066
98. LP (1) N 44	/834. BD*(1)Se 1 - C 4	0.72	0.61	0.019
98. LP (1) N 44	/840. BD*(1) C 4 - C 7	0.14	1.01	0.011
98. LP (1) N 44	/843. BD*(1) C 5 - C 9	0.07	1.03	0.008

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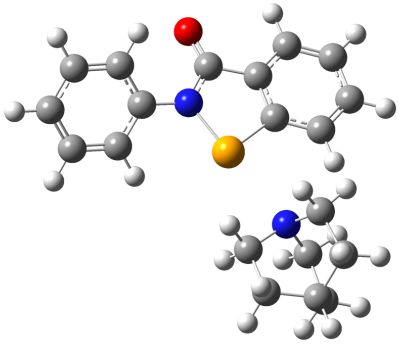
1a.quinuclidine



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1	Se			
2	O	3.9585573		
3	N	1.8847897	21.0234737	
4	C	1.8876581	85.5795207	-2.2531818
5	C	1.3883527	127.6875975	-179.0092638
6	H	1.0790357	120.8479720	0.2973914
7	C	1.3879752	111.7978252	0.8539788
8	C	1.2149130	12.0663076	-176.2636838
9	C	1.3834555	118.6671509	-179.9192945
10	H	1.0829912	119.2220094	179.9602690
11	C	1.4126380	119.1361146	-178.9688768
12	C	1.3936717	121.1012305	-0.1437456
13	H	1.0820633	119.8958861	-179.9301380
14	C	1.3809471	119.8850517	-0.0372151
15	H	1.0827134	122.0416434	-179.8107492
16	C	1.3925271	120.9070090	137.5848597
17	H	1.0792815	119.6336740	2.0493834
18	C	1.3918649	119.5759146	-41.1577701
19	H	1.0830423	119.7090272	-2.8086007
20	C	1.3854623	120.2707793	178.1976196
21	H	1.0826965	119.4778468	-179.9736850
22	C	1.3841350	119.7372849	-178.8944278
23	H	1.0827169	119.1834757	-179.6678662
24	C	1.3852240	120.2762287	0.7666040
25	H	1.0823361	120.3022756	179.5440087
26	C	3.2227541	151.4398759	175.3667782
27	C	2.3900331	79.7191056	-143.4421273
28	C	2.3887707	82.3239914	155.5075620

29	C	1.5475413	169.1360960	-134.5646652
30	H	1.0916504	67.9750864	-46.7133345
31	H	1.0917801	78.8524337	67.0715294
32	H	1.0910270	143.5396344	-40.0279818
33	H	1.0911196	86.9343155	74.6252048
34	C	1.5489418	93.7153216	-174.0720740
35	C	1.5491044	89.4357762	177.1166810
36	H	1.0912057	143.4368704	51.8895836
37	H	1.0910023	92.3291049	-71.2784560
38	C	1.5304627	107.9792474	-44.8972342
39	H	1.0920750	110.8278362	75.4907062
40	H	1.0915274	110.7027964	-165.7869388
41	H	1.0922743	110.8395917	144.1120862
42	H	1.0915266	110.7150502	-97.1749576
43	H	1.0916104	110.6961002	-156.9414957
44	H	1.0921367	110.8458465	84.3463784
45	H	1.0904117	110.3195158	-175.6801394
46	N	1.4659554	35.4728577	47.2128401

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
1. BD (1)Se 1 - N 3	/812. RY*(1) N 46	0.72	1.73	0.032
2. BD (1)Se 1 - C 4	/812. RY*(1) N 46	0.26	1.71	0.019
10. BD (1) C 5 - H 6	/875. BD*(1) C 26 - N 46	0.13	1.02	0.010
10. BD (1) C 5 - H 6	/876. BD*(1) C 27 - H 32	0.07	1.06	0.008
10. BD (1) C 5 - H 6	/880. BD*(1) C 28 - C 35	0.10	1.02	0.009
10. BD (1) C 5 - H 6	/881. BD*(1) C 28 - H 36	0.10	1.06	0.009
94. LP (1)Se 1	/812. RY*(1) N 46	0.06	1.82	0.009
94. LP (1)Se 1	/872. BD*(1) C 26 - C 29	0.82	1.20	0.028
94. LP (1)Se 1	/879. BD*(1) C 27 - N 46	0.39	1.20	0.019
94. LP (1)Se 1	/883. BD*(1) C 28 - N 46	0.54	1.20	0.023
95. LP (2)Se 1	/873. BD*(1) C 26 - H 30	0.14	0.75	0.009
95. LP (2)Se 1	/878. BD*(1) C 27 - C 34	0.14	0.71	0.009
95. LP (2)Se 1	/879. BD*(1) C 27 - N 46	0.14	0.71	0.009
95. LP (2)Se 1	/880. BD*(1) C 28 - C 35	0.08	0.71	0.007
95. LP (2)Se 1	/883. BD*(1) C 28 - N 46	0.18	0.71	0.010
from unit 2 to unit 1				
36. BD (1) C 26 - H 30	/100. RY*(1)Se 1	0.08	1.41	0.009
36. BD (1) C 26 - H 30	/103. RY*(4)Se 1	0.18	1.70	0.016
36. BD (1) C 26 - H 30	/838. BD*(1)Se 1 - N 3	0.11	0.74	0.008
36. BD (1) C 26 - H 30	/839. BD*(1)Se 1 - C 4	0.18	0.80	0.011
37. BD (1) C 26 - H 31	/103. RY*(4)Se 1	0.10	1.70	0.012
37. BD (1) C 26 - H 31	/106. RY*(7)Se 1	0.05	2.01	0.009
37. BD (1) C 26 - H 31	/838. BD*(1)Se 1 - N 3	0.06	0.74	0.006
37. BD (1) C 26 - H 31	/839. BD*(1)Se 1 - C 4	0.05	0.80	0.006
38. BD (1) C 26 - N 46	/838. BD*(1)Se 1 - N 3	0.15	0.95	0.011
39. BD (1) C 27 - H 32	/234. RY*(1) H 6	0.16	1.57	0.014
39. BD (1) C 27 - H 32	/847. BD*(1) C 5 - H 6	0.18	1.08	0.012
39. BD (1) C 27 - H 32	/849. BD*(2) C 5 - C 9	0.06	0.67	0.006
40. BD (1) C 27 - H 33	/104. RY*(5)Se 1	0.08	1.68	0.010
40. BD (1) C 27 - H 33	/105. RY*(6)Se 1	0.07	2.04	0.011
40. BD (1) C 27 - H 33	/106. RY*(7)Se 1	0.09	2.01	0.012
41. BD (1) C 27 - C 34	/838. BD*(1)Se 1 - N 3	0.09	0.84	0.008
42. BD (1) C 27 - N 46	/838. BD*(1)Se 1 - N 3	0.09	0.95	0.009

43. BD (1) C 28 - C 35	/838. BD*(1)Se 1 - N 3	0.10	0.84	0.008
44. BD (1) C 28 - H 36	/234. RY*(1) H 6	0.30	1.57	0.019
44. BD (1) C 28 - H 36	/847. BD*(1) C 5 - H 6	0.44	1.08	0.020
45. BD (1) C 28 - H 37	/104. RY*(5)Se 1	0.05	1.68	0.009
45. BD (1) C 28 - H 37	/105. RY*(6)Se 1	0.09	2.04	0.012
45. BD (1) C 28 - H 37	/107. RY*(8)Se 1	0.06	2.13	0.010
46. BD (1) C 28 - N 46	/838. BD*(1)Se 1 - N 3	0.08	0.95	0.008
46. BD (1) C 28 - N 46	/847. BD*(1) C 5 - H 6	0.07	1.29	0.009
93. CR (1) N 46	/838. BD*(1)Se 1 - N 3	0.06	14.42	0.027
99. LP (1) N 46	/100. RY*(1)Se 1	0.18	1.21	0.014
99. LP (1) N 46	/101. RY*(2)Se 1	0.94	1.47	0.034
99. LP (1) N 46	/103. RY*(4)Se 1	0.06	1.50	0.009
99. LP (1) N 46	/106. RY*(7)Se 1	0.07	1.81	0.010
99. LP (1) N 46	/110. RY*(11)Se 1	0.06	1.88	0.010
99. LP (1) N 46	/116. RY*(17)Se 1	0.06	2.76	0.012
99. LP (1) N 46	/838. BD*(1)Se 1 - N 3	10.11	0.54	0.067
99. LP (1) N 46	/839. BD*(1)Se 1 - C 4	0.76	0.60	0.020
99. LP (1) N 46	/845. BD*(1) C 4 - C 7	0.14	1.00	0.011
99. LP (1) N 46	/848. BD*(1) C 5 - C 9	0.07	1.03	0.008

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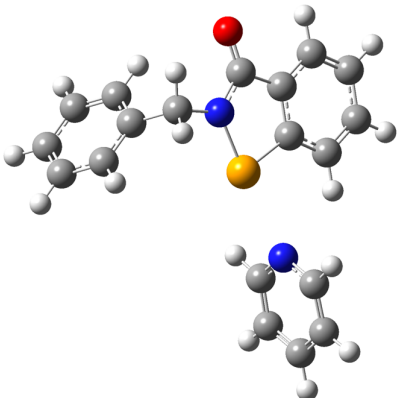
1b.pyridine



Sum of electronic and zero-point Energies= -3319.713802
Sum of electronic and thermal Energies= -3319.693712
Sum of electronic and thermal Enthalpies= -3319.692767
Sum of electronic and thermal Free Energies= -3319.769696

1	O			
2	N	2.2873562		
3	C	2.5506623	95.5093419	
4	C	1.3893855	174.7226394	173.8096095
5	H	1.0800564	120.7639763	8.3037486
6	C	1.3896179	64.6683257	1.6439913
7	C	1.4479618	96.0274283	-178.5274035
8	H	1.0914637	105.8435910	-16.5933680
9	H	1.0929702	109.2840874	-132.6690412
10	C	1.2193930	29.3764399	-178.6152959
11	C	1.3838154	118.4834662	-171.7745820
12	H	1.0830616	119.1159836	179.9645153
13	C	1.5097880	113.1236501	104.2247606
14	C	1.3938550	121.2571604	-0.0730922
15	H	1.0821706	119.9000386	-179.9574391
16	C	1.3809053	119.8857438	0.0102732
17	H	1.0827649	122.0576226	-179.8725106
18	C	1.3874091	121.1107362	118.8333959
19	H	1.0844699	119.5789242	0.2172248

20	C	1.3922827	119.8013127	-60.7804692
21	H	1.0840223	119.2045880	-0.6693524
22	C	1.3837536	120.3960997	179.5626839
23	H	1.0828500	119.7925549	179.8480237
24	C	1.3885530	120.6305296	-179.6784822
25	H	1.0828626	119.8760846	179.9760548
26	C	1.3846525	119.9621317	0.1467390
27	H	1.0827530	120.1540472	179.9573434
28	Se	1.8661094	143.1206429	-4.7919762
29	N	2.8081066	175.7518337	-12.4614980
30	C	1.3294958	122.7123448	115.7156880
31	C	1.3295854	116.6379334	-82.1609029
32	C	1.3851991	122.9996051	161.9862884
33	H	1.0847336	116.0733309	-17.9660900
34	C	1.3852260	122.9715030	-163.1213346
35	H	1.0847542	116.0188375	16.7348808
36	C	1.3849819	118.4855597	0.1114371
37	H	1.0815596	120.2000014	-179.9730892
38	H	1.0815280	120.1718040	-179.9871179
39	H	1.0826581	120.5924592	179.9435308

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
5. BD (1) N 2 -Se 28	/595. RY*(1) N 29	0.54	1.88	0.029
6. BD (1) C 3 - C 4	/598. RY*(4) N 29	0.07	1.65	0.010
9. BD (1) C 3 -Se 28	/595. RY*(1) N 29	0.22	1.85	0.018
10. BD (1) C 4 - H 5	/815. BD*(2) N 29 - C 31	0.20	0.64	0.011
91. LP (1)Se 28	/595. RY*(1) N 29	0.10	1.95	0.013
91. LP (1)Se 28	/813. BD*(1) N 29 - C 30	0.47	1.37	0.023
91. LP (1)Se 28	/814. BD*(1) N 29 - C 31	0.35	1.37	0.020
91. LP (1)Se 28	/815. BD*(2) N 29 - C 31	0.22	0.81	0.013
92. LP (2)Se 28	/813. BD*(1) N 29 - C 30	0.18	0.89	0.012
92. LP (2)Se 28	/814. BD*(1) N 29 - C 31	0.12	0.89	0.010
92. LP (2)Se 28	/816. BD*(1) C 30 - C 32	0.07	0.90	0.007
92. LP (2)Se 28	/819. BD*(1) C 31 - C 34	0.12	0.90	0.010
from unit 2 to unit 1				
38. BD (1) N 29 - C 30	/780. BD*(1) N 2 -Se 28	0.12	1.12	0.011
39. BD (1) N 29 - C 31	/780. BD*(1) N 2 -Se 28	0.13	1.12	0.011
40. BD (2) N 29 - C 31	/199. RY*(2) H 5	0.05	2.83	0.012
40. BD (2) N 29 - C 31	/780. BD*(1) N 2 -Se 28	0.15	0.55	0.009
40. BD (2) N 29 - C 31	/785. BD*(1) C 4 - H 5	0.15	0.88	0.011
41. BD (1) C 30 - C 32	/780. BD*(1) N 2 -Se 28	0.13	1.00	0.010
44. BD (1) C 31 - C 34	/780. BD*(1) N 2 -Se 28	0.12	1.00	0.010
93. LP (1) N 29	/176. RY*(5) C 4	0.06	2.23	0.010
93. LP (1) N 29	/199. RY*(2) H 5	0.05	2.90	0.011
93. LP (1) N 29	/566. RY*(2)Se 28	0.72	1.61	0.031
93. LP (1) N 29	/569. RY*(5)Se 28	0.09	1.49	0.011
93. LP (1) N 29	/780. BD*(1) N 2 -Se 28	9.69	0.62	0.070
93. LP (1) N 29	/782. BD*(1) C 3 - C 6	0.27	1.07	0.015
93. LP (1) N 29	/784. BD*(1) C 3 -Se 28	0.53	0.66	0.017
93. LP (1) N 29	/785. BD*(1) C 4 - H 5	0.30	0.95	0.015
93. LP (1) N 29	/786. BD*(1) C 4 - C 11	0.22	1.10	0.014
815. BD*(2) N 29 - C 31	/780. BD*(1) N 2 -Se 28	0.16	0.14	0.009
815. BD*(2) N 29 - C 31	/785. BD*(1) C 4 - H 5	0.09	0.46	0.013

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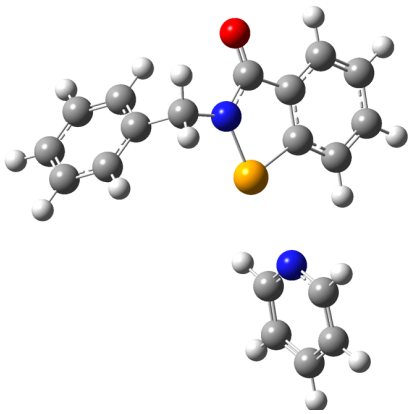
1b.DMAP



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1	O			
2	N	2.2873562		
3	C	2.5506623	95.5093419	
4	C	1.3893855	174.7226394	173.8096095
5	H	1.0800564	120.7639763	8.3037486
6	C	1.3896179	64.6683257	1.6439913
7	C	1.4479618	96.0274283	-178.5274035
8	H	1.0914637	105.8435910	-16.5933680
9	H	1.0929702	109.2840874	-132.6690412
10	C	1.2193930	29.3764399	-178.6152959
11	C	1.3838154	118.4834662	-171.7745820
12	H	1.0830616	119.1159836	179.9645153
13	C	1.5097880	113.1236501	104.2247606
14	C	1.3938550	121.2571604	-0.0730922
15	H	1.0821706	119.9000386	-179.9574391
16	C	1.3809053	119.8857438	0.0102732
17	H	1.0827649	122.0576226	-179.8725106
18	C	1.3874091	121.1107362	118.8333959
19	H	1.0844699	119.5789242	0.2172248
20	C	1.3922827	119.8013127	-60.7804692
21	H	1.0840223	119.2045880	-0.6693524
22	C	1.3837536	120.3960997	179.5626839
23	H	1.0828500	119.7925549	179.8480237
24	C	1.3885530	120.6305296	-179.6784822
25	H	1.0828626	119.8760846	179.9760548
26	C	1.3846525	119.9621317	0.1467390
27	H	1.0827530	120.1540472	179.9573434
28	Se	1.8661094	143.1206429	-4.7919762
29	N	2.8081066	175.7518337	-12.4614980
30	C	1.3294958	122.7123448	115.7156880
31	C	1.3295854	116.6379334	-82.1609029
32	C	1.3851991	122.9996051	161.9862884
33	H	1.0847336	116.0733309	-17.9660900
34	C	1.3852260	122.9715030	-163.1213346

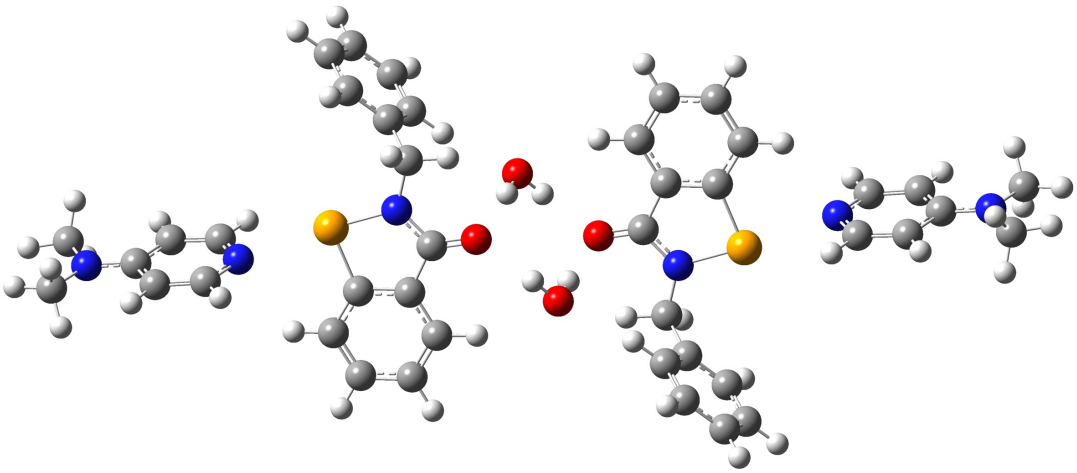
35	H	1.0847542	116.0188375	16.7348808
36	C	1.3849819	118.4855597	0.1114371
37	H	1.0815596	120.2000014	-179.9730892
38	H	1.0815280	120.1718040	-179.9871179
39	H	1.0826581	120.5924592	179.9435308

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
5. BD (1) N 2 -Se 28	/608. RY*(1) N 29	0.64	1.88	0.031
5. BD (1) N 2 -Se 28	/610. RY*(3) N 29	0.08	1.52	0.010
6. BD (1) C 3 - C 4	/608. RY*(1) N 29	0.05	1.99	0.009
6. BD (1) C 3 - C 4	/610. RY*(3) N 29	0.06	1.63	0.009
9. BD (1) C 3 -Se 28	/608. RY*(1) N 29	0.27	1.85	0.020
10. BD (1) C 4 - H 5	/104. LP (2) N 29	0.46	0.38	0.019
77. CR (3)Se 28	/929. BD*(1) N 29 - C 30	0.06	11.37	0.023
101. LP (1)Se 28	/104. LP (2) N 29	0.34	0.56	0.020
101. LP (1)Se 28	/608. RY*(1) N 29	0.13	1.96	0.014
101. LP (1)Se 28	/929. BD*(1) N 29 - C 30	0.59	1.38	0.025
101. LP (1)Se 28	/930. BD*(1) N 29 - C 31	0.45	1.38	0.022
102. LP (2)Se 28	/929. BD*(1) N 29 - C 30	0.22	0.89	0.013
102. LP (2)Se 28	/930. BD*(1) N 29 - C 31	0.17	0.89	0.012
102. LP (2)Se 28	/931. BD*(1) C 30 - C 32	0.09	0.92	0.008
102. LP (2)Se 28	/934. BD*(1) C 31 - C 34	0.12	0.92	0.010
from unit 2 to unit 1				
38. BD (1) N 29 - C 30	/896. BD*(1) N 2 -Se 28	0.17	1.10	0.012
39. BD (1) N 29 - C 31	/896. BD*(1) N 2 -Se 28	0.17	1.10	0.013
40. BD (1) C 30 - C 32	/896. BD*(1) N 2 -Se 28	0.15	0.99	0.011
41. BD (2) C 30 - C 32	/211. RY*(1) H 5	0.05	1.18	0.008
43. BD (1) C 31 - C 34	/896. BD*(1) N 2 -Se 28	0.15	0.99	0.011
89. CR (1) N 29	/896. BD*(1) N 2 -Se 28	0.08	14.40	0.030
103. LP (1) N 29	/189. RY*(5) C 4	0.08	2.23	0.012
103. LP (1) N 29	/212. RY*(2) H 5	0.06	2.91	0.012
103. LP (1) N 29	/579. RY*(2)Se 28	0.94	1.63	0.036
103. LP (1) N 29	/582. RY*(5)Se 28	0.12	1.47	0.012
103. LP (1) N 29	/583. RY*(6)Se 28	0.06	1.57	0.009
103. LP (1) N 29	/586. RY*(9)Se 28	0.05	2.01	0.009
103. LP (1) N 29	/896. BD*(1) N 2 -Se 28	12.79	0.61	0.080
103. LP (1) N 29	/898. BD*(1) C 3 - C 6	0.32	1.06	0.017
103. LP (1) N 29	/900. BD*(1) C 3 -Se 28	0.77	0.65	0.021
103. LP (1) N 29	/901. BD*(1) C 4 - H 5	0.29	0.95	0.015
103. LP (1) N 29	/902. BD*(1) C 4 - C 11	0.25	1.09	0.015
104. LP (2) N 29	/896. BD*(1) N 2 -Se 28	0.39	0.39	0.013
104. LP (2) N 29	/901. BD*(1) C 4 - H 5	0.39	0.72	0.019
104. LP (2) N 29	/902. BD*(1) C 4 - C 11	0.08	0.87	0.009
932. BD*(2) C 30 - C 32	/903. BD*(2) C 4 - C 11	0.10	0.02	0.002
935. BD*(2) C 31 - C 34	/903. BD*(2) C 4 - C 11	0.08	0.02	0.002

1b.DMAP.H_2O



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C	3.429821	1.462522	-0.582959
C	4.771111	3.69886	0.312442
H	5.293802	4.579673	0.665135
N	3.758485	-0.749056	-1.202817
C	3.387876	3.737547	0.146878
H	2.841197	4.643388	0.374016
C	3.453046	-2.081703	-1.694819
H	3.864872	-2.197909	-2.701673
H	2.367186	-2.138913	-1.77067
O	1.62388	0.042791	-1.314282
C	5.493651	2.550726	0.043078
H	6.563358	2.520117	0.187854
C	3.986447	-3.16545	-0.791183
C	5.575085	-4.924556	-0.343683
H	6.417218	-5.526233	-0.66241
C	2.711216	2.619619	-0.298996
H	1.633655	2.624346	-0.413591
C	4.810455	1.428298	-0.40762
C	3.411831	-3.377335	0.459457
H	2.557478	-2.783032	0.76882
C	5.065886	-3.945121	-1.185103
H	5.515145	-3.783945	-2.159069

C	5.0033	-5.128637	0.901186
H	5.396193	-5.89261	1.560709
C	3.920631	-4.354413	1.298233
H	3.464768	-4.516068	2.267075
C	2.821628	0.209852	-1.063676
O	0.54424	-1.705949	0.682679
H	-0.136015	-1.168207	1.114165
H	0.816914	-1.173904	-0.078075
C	10.231981	1.257194	-0.840416
H	10.835114	1.74587	-1.590429
C	10.801541	0.708025	0.323274
C	9.907532	0.088271	1.215135
H	10.247485	-0.370529	2.131073
N	8.028849	0.587015	-0.182948
C	13.025816	1.365386	-0.403506
H	13.004212	0.827927	-1.357415
H	14.043798	1.337086	-0.023711
H	12.769274	2.411397	-0.593693
C	8.871274	1.168614	-1.03413
H	8.426312	1.590513	-1.929565
C	8.563221	0.05862	0.915963
H	7.868704	-0.42223	1.59709
C	12.685187	0.142908	1.751421
H	12.253058	0.562211	2.664346
H	13.758114	0.313702	1.783039
H	12.512944	-0.938517	1.755612
N	12.137794	0.771972	0.570516
Se	-5.545859	0.259516	0.852708
C	-3.436671	-1.468279	0.65696
C	-4.750616	-3.695972	-0.29962
H	-5.262149	-4.573392	-0.676318
N	-3.786609	0.735599	1.293636
C	-3.372307	-3.734893	-0.097076
H	-2.818464	-4.63752	-0.319624
C	-3.497067	2.063233	1.807884
H	-3.932253	2.166681	2.806276
H	-2.413408	2.122735	1.909385
O	-1.653552	-0.052285	1.450281
C	-5.481728	-2.551695	-0.036977
H	-6.54711	-2.520117	-0.21062
C	-4.013307	3.15576	0.90485
C	-5.594515	4.918145	0.444108
H	-6.443419	5.515791	0.752281
C	-2.709227	-2.6214	0.379409
H	-1.635077	-2.626429	0.522479
C	-4.812125	-1.433948	0.4447

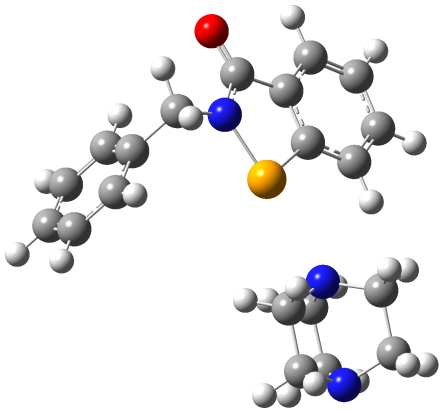
C	-3.414326	3.380841	-0.331984
H	-2.553782	2.789998	-0.630704
C	-5.101115	3.93045	1.28529
H	-5.569545	3.758749	2.248358
C	-4.998444	5.135456	-0.787032
H	-5.37898	5.905866	-1.446316
C	-3.907428	4.366103	-1.170551
H	-3.43278	4.53791	-2.12857
C	-2.843955	-0.219895	1.167583
O	-0.54962	1.709187	-0.5213
H	0.124322	1.164179	-0.954004
H	-0.830079	1.177482	0.236788
C	-10.262633	-1.262019	0.660576
H	-10.902053	-1.761269	1.372637
C	-10.774621	-0.694653	-0.520965
C	-9.838101	-0.062298	-1.358597
H	-10.133153	0.410847	-2.282757
N	-8.029778	-0.584307	0.121591
C	-13.031983	-1.360112	0.086498
H	-13.056511	-0.837003	1.048313
H	-14.030246	-1.324886	-0.341952
H	-12.78552	-2.409154	0.273297
C	-8.912826	-1.178036	0.921657
H	-8.512308	-1.614032	1.831202
C	-8.509959	-0.038757	-0.993835
H	-7.782944	0.451765	-1.632927
C	-12.585922	-0.105065	-2.030215
H	-12.109155	-0.509906	-2.927304
H	-13.655967	-0.274635	-2.117474
H	-12.413765	0.976186	-2.008572
N	-12.097259	-0.753439	-0.834129

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
210.LP (1)N 37.	/***.BD*(1)Se 1 -N 5.	13.51	0.61	0.082

1b.DABCO



Sum of electronic and zero-point Energies= -3416.687566
Sum of electronic and thermal Energies= -3416.665539
Sum of electronic and thermal Enthalpies= -3416.664595
Sum of electronic and thermal Free Energies= -3416.744396

1	O			
2	N	2.2885304		
3	C	2.5461805	95.5249623	
4	C	1.3881234	174.3360128	165.8635744
5	H	1.0795435	120.7711088	15.9548145
6	C	1.3890925	64.8320922	1.8332635
7	C	1.4475188	96.3104039	-178.2217161
8	H	1.0914039	105.7510470	-10.8198382
9	H	1.0932866	109.4948649	-126.9439460
10	C	1.2185939	29.3477433	-178.2159397
11	C	1.3835841	118.5924476	-163.6482515
12	H	1.0830202	119.2414707	179.9153580
13	C	1.5096143	112.7983113	110.0984282
14	C	1.3938673	121.1118213	0.0628704
15	H	1.0820911	119.8625554	179.9979071
16	C	1.3813352	119.9405040	0.2187552
17	H	1.0827655	122.0061005	179.7699631
18	C	1.3874767	121.0948098	118.2667405
19	H	1.0845003	119.5482429	0.7745543
20	C	1.3920184	119.8299393	-60.8339906
21	H	1.0840822	119.2232361	-0.9549631
22	C	1.3835849	120.4364178	179.0654933
23	H	1.0828015	119.8197953	179.8389958
24	C	1.3886494	120.6298245	-179.1483700
25	H	1.0828729	119.8833252	-179.9482986
26	C	1.3846754	119.9597318	0.1369325
27	H	1.0826998	120.1546510	179.9802893
28	C	3.8005758	98.4704369	7.5958629
29	C	2.3923609	69.1952574	81.9963680
30	C	2.3837244	98.3692348	28.7128219
31	C	1.5548116	149.4793962	132.1403256
32	H	1.0917198	49.4981677	-169.0800464
33	H	1.0913611	97.6184192	-62.6808793
34	H	1.0913242	143.1652551	-76.5024662
35	H	1.0915044	90.8183852	44.5086496

36	C	1.5539830	89.4525412	155.9384513
37	C	1.5528218	90.2426709	149.3721598
38	H	1.0919829	143.7065071	20.5447882
39	H	1.0920580	89.3779152	-98.9832092
40	H	1.0916345	111.2037088	45.3251506
41	H	1.0916047	111.2173086	165.0721870
42	H	1.0914920	111.2251178	151.0752789
43	H	1.0916667	111.2505860	-89.1530574
44	H	1.0915126	111.2005660	-149.1643067
45	H	1.0915990	111.2531469	91.0529840
46	Se	1.8669559	142.9991024	-6.2789178
47	N	1.4650621	65.9579847	43.8542916
48	N	1.4595290	110.0408545	-74.8489168

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
5. BD (1) N 2 -Se 46	/821. RY*(1) N 47	0.57	1.75	0.028
9. BD (1) C 3 -Se 46	/821. RY*(1) N 47	0.24	1.72	0.018
10. BD (1) C 4 - H 5	/910. BD*(1) C 28 - C 31	0.07	1.01	0.008
10. BD (1) C 4 - H 5	/911. BD*(1) C 28 - H 32	0.09	1.05	0.009
10. BD (1) C 4 - H 5	/915. BD*(1) C 29 - H 35	0.05	1.06	0.007
10. BD (1) C 4 - H 5	/921. BD*(1) C 30 - N 47	0.13	1.02	0.010
100. LP (1)Se 46	/821. RY*(1) N 47	0.05	1.82	0.009
100. LP (1)Se 46	/913. BD*(1) C 28 - N 47	0.57	1.19	0.023
100. LP (1)Se 46	/917. BD*(1) C 29 - N 47	0.29	1.19	0.017
100. LP (1)Se 46	/918. BD*(1) C 30 - C 37	0.74	1.18	0.027
101. LP (2)Se 46	/910. BD*(1) C 28 - C 31	0.05	0.69	0.006
101. LP (2)Se 46	/913. BD*(1) C 28 - N 47	0.23	0.71	0.012
101. LP (2)Se 46	/916. BD*(1) C 29 - C 36	0.16	0.69	0.010
101. LP (2)Se 46	/917. BD*(1) C 29 - N 47	0.08	0.71	0.007
101. LP (2)Se 46	/919. BD*(1) C 30 - H 38	0.14	0.75	0.010
from unit 2 to unit 1				
38. BD (1) C 28 - C 31	/877. BD*(1) N 2 -Se 46	0.10	0.85	0.008
39. BD (1) C 28 - H 32	/208. RY*(1) H 5	0.36	1.57	0.021
39. BD (1) C 28 - H 32	/882. BD*(1) C 4 - H 5	0.41	1.09	0.019
40. BD (1) C 28 - H 33	/795. RY*(5)Se 46	0.06	1.73	0.009
40. BD (1) C 28 - H 33	/799. RY*(9)Se 46	0.07	1.93	0.010
41. BD (1) C 28 - N 47	/882. BD*(1) C 4 - H 5	0.07	1.29	0.008
42. BD (1) C 29 - H 34	/791. RY*(1)Se 46	0.05	1.36	0.008
42. BD (1) C 29 - H 34	/795. RY*(5)Se 46	0.17	1.72	0.015
42. BD (1) C 29 - H 34	/798. RY*(8)Se 46	0.05	2.58	0.011
43. BD (1) C 29 - H 35	/184. RY*(3) C 4	0.06	1.27	0.008
43. BD (1) C 29 - H 35	/208. RY*(1) H 5	0.11	1.56	0.011
43. BD (1) C 29 - H 35	/882. BD*(1) C 4 - H 5	0.10	1.08	0.009
43. BD (1) C 29 - H 35	/884. BD*(2) C 4 - C 11	0.07	0.67	0.007
44. BD (1) C 29 - C 36	/877. BD*(1) N 2 -Se 46	0.07	0.85	0.007
45. BD (1) C 29 - N 47	/877. BD*(1) N 2 -Se 46	0.08	0.96	0.008
47. BD (1) C 30 - H 38	/791. RY*(1)Se 46	0.08	1.36	0.009
47. BD (1) C 30 - H 38	/794. RY*(4)Se 46	0.11	1.90	0.013
47. BD (1) C 30 - H 38	/877. BD*(1) N 2 -Se 46	0.09	0.76	0.008
47. BD (1) C 30 - H 38	/881. BD*(1) C 3 -Se 46	0.14	0.80	0.010
48. BD (1) C 30 - H 39	/794. RY*(4)Se 46	0.08	1.90	0.011
49. BD (1) C 30 - N 47	/877. BD*(1) N 2 -Se 46	0.10	0.96	0.009
102. LP (1) N 47	/792. RY*(2)Se 46	0.90	1.42	0.033

102. LP (1) N 47	/794. RY*(4)Se 46	0.06	1.70	0.009
102. LP (1) N 47	/795. RY*(5)Se 46	0.18	1.53	0.015
102. LP (1) N 47	/797. RY*(7)Se 46	0.07	1.62	0.010
102. LP (1) N 47	/806. RY*(16)Se 46	0.07	2.43	0.012
102. LP (1) N 47	/807. RY*(17)Se 46	0.05	2.34	0.010
102. LP (1) N 47	/877. BD*(1) N 2 -Se 46	8.11	0.56	0.061
102. LP (1) N 47	/879. BD*(1) C 3 - C 6	0.13	1.00	0.011
102. LP (1) N 47	/881. BD*(1) C 3 -Se 46	0.66	0.60	0.018
102. LP (1) N 47	/883. BD*(1) C 4 - C 11	0.07	1.03	0.008

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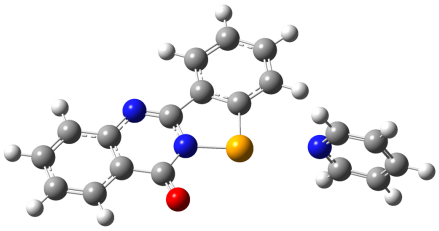
3.pyridine



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Sum of electronic and thermal Enthalpies= -3372.685988
Sum of electronic and thermal Free Energies= -3372.758608

1	Se			
2	C	4.0945945		
3	H	1.0822296	132.0415320	
4	N	1.8784552	63.1075590	-0.1466880
5	C	1.3901911	13.3133129	-0.0138634
6	C	1.3797807	106.0054721	179.8743725
7	H	1.0820298	120.1219820	179.9687255
8	C	1.3832129	119.0614248	179.9217645
9	C	1.3947042	120.6361630	0.1075609
10	C	2.4761502	141.9561784	-179.8783000
11	H	1.0822248	87.5940048	-179.9620351
12	N	2.3535426	143.9126364	0.2695521
13	O	1.2158337	120.4550473	0.1238177
14	C	2.3993256	120.3115264	0.0480718
15	H	1.0830887	149.3832785	179.9811865
16	C	1.3896573	120.0423030	0.0679948
17	H	1.0798686	120.5331308	179.8675356
18	C	1.3765931	88.0254038	179.7803379
19	C	1.2893984	28.5782273	-0.2124444
20	C	1.3734973	150.7709991	0.0606224
21	H	1.0821270	120.2609601	179.9752419
22	C	1.3835345	118.8614162	-0.0688095
23	H	1.0829038	119.1281235	179.9971482
24	C	1.3732464	91.0339728	-0.0150706
25	H	1.0819884	121.5642423	179.9963581
26	C	1.3983215	30.6962268	0.0211644
27	N	2.7647396	175.0127404	-6.2613025
28	C	1.3297677	119.0664140	-90.6339476
29	C	1.3296713	119.8424149	108.4889355
30	C	1.3848136	122.9375832	-161.4174878
31	H	1.0846567	116.0803408	18.4136625
32	C	1.3849551	122.9263103	161.2638736
33	H	1.0845882	116.0949181	-18.5547894

34	C	1.3850146	118.4828824	-0.1145477
35	H	1.0814627	120.1698186	179.9329318
36	H	1.0814710	120.1639365	-179.9417357
37	H	1.0826096	120.5756889	-179.8913610

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
1. BD (1)Se 1 - N 4	/607. RY*(1) N 27	0.54	1.89	0.029
1. BD (1)Se 1 - N 4	/609. RY*(3) N 27	0.05	1.89	0.009
2. BD (2)Se 1 - N 4	/608. RY*(2) N 27	0.11	1.32	0.012
3. BD (1)Se 1 - C 9	/607. RY*(1) N 27	0.22	1.85	0.018
18. BD (1) C 9 - C 16	/610. RY*(4) N 27	0.08	1.66	0.010
30. BD (1) C 16 - H 17	/828. BD*(2) N 27 - C 29	0.22	0.64	0.012
90. LP (1)Se 1	/607. RY*(1) N 27	0.08	1.97	0.012
90. LP (1)Se 1	/826. BD*(1) N 27 - C 28	0.46	1.39	0.023
90. LP (1)Se 1	/827. BD*(1) N 27 - C 29	0.46	1.39	0.023
90. LP (1)Se 1	/828. BD*(2) N 27 - C 29	0.28	0.82	0.015
91. LP (2)Se 1	/608. RY*(2) N 27	1.54	0.98	0.042
91. LP (2)Se 1	/613. RY*(7) N 27	0.20	5.07	0.034
91. LP (2)Se 1	/615. RY*(9) N 27	0.19	2.08	0.021
91. LP (2)Se 1	/618. RY*(12) N 27	0.08	3.68	0.019
91. LP (2)Se 1	/633. RY*(1) C 28	0.10	1.56	0.014
91. LP (2)Se 1	/634. RY*(2) C 28	0.38	1.40	0.025
91. LP (2)Se 1	/635. RY*(3) C 28	0.05	0.89	0.007
91. LP (2)Se 1	/636. RY*(4) C 28	0.08	1.50	0.012
91. LP (2)Se 1	/639. RY*(7) C 28	0.09	2.08	0.015
91. LP (2)Se 1	/645. RY*(13) C 28	0.09	2.05	0.015
91. LP (2)Se 1	/659. RY*(1) C 29	0.11	1.56	0.014
91. LP (2)Se 1	/660. RY*(2) C 29	0.32	1.40	0.023
91. LP (2)Se 1	/662. RY*(4) C 29	0.05	1.50	0.010
91. LP (2)Se 1	/665. RY*(7) C 29	0.09	2.11	0.015
91. LP (2)Se 1	/670. RY*(12) C 29	0.10	1.83	0.015
91. LP (2)Se 1	/826. BD*(1) N 27 - C 28	0.14	0.57	0.010
91. LP (2)Se 1	/827. BD*(1) N 27 - C 29	0.15	0.58	0.010
91. LP (2)Se 1	/828. BD*(2) N 27 - C 29	0.79	0.01	0.003
91. LP (2)Se 1	/829. BD*(1) C 28 - C 30	0.14	0.59	0.010
91. LP (2)Se 1	/830. BD*(2) C 28 - C 30	0.30	0.04	0.003
91. LP (2)Se 1	/831. BD*(1) C 28 - H 31	0.06	0.44	0.006
91. LP (2)Se 1	/832. BD*(1) C 29 - C 32	0.13	0.59	0.009
91. LP (2)Se 1	/833. BD*(1) C 29 - H 33	0.06	0.44	0.005
789. BD*(2)Se 1 - N 4	/608. RY*(2) N 27	2.71	0.37	0.058
789. BD*(2)Se 1 - N 4	/613. RY*(7) N 27	0.19	4.46	0.054
789. BD*(2)Se 1 - N 4	/615. RY*(9) N 27	0.39	1.47	0.044
789. BD*(2)Se 1 - N 4	/618. RY*(12) N 27	0.10	3.08	0.033
789. BD*(2)Se 1 - N 4	/633. RY*(1) C 28	0.17	0.95	0.024
789. BD*(2)Se 1 - N 4	/634. RY*(2) C 28	0.26	0.80	0.026
789. BD*(2)Se 1 - N 4	/635. RY*(3) C 28	0.09	0.28	0.009
789. BD*(2)Se 1 - N 4	/636. RY*(4) C 28	0.18	0.90	0.023
789. BD*(2)Se 1 - N 4	/639. RY*(7) C 28	0.12	1.47	0.025
789. BD*(2)Se 1 - N 4	/645. RY*(13) C 28	0.11	1.44	0.024
789. BD*(2)Se 1 - N 4	/646. RY*(14) C 28	0.06	1.51	0.018
789. BD*(2)Se 1 - N 4	/659. RY*(1) C 29	0.18	0.95	0.024
789. BD*(2)Se 1 - N 4	/660. RY*(2) C 29	0.20	0.80	0.023
789. BD*(2)Se 1 - N 4	/661. RY*(3) C 29	0.08	0.34	0.009
789. BD*(2)Se 1 - N 4	/662. RY*(4) C 29	0.13	0.90	0.020

789. BD*(2)Se 1 - N 4	/665. RY*(7) C 29	0.13	1.50	0.025
789. BD*(2)Se 1 - N 4	/670. RY*(12) C 29	0.14	1.22	0.024
789. BD*(2)Se 1 - N 4	/677. RY*(19) C 29	0.06	1.61	0.018
789. BD*(2)Se 1 - N 4	/686. RY*(2) C 30	0.06	0.92	0.014
789. BD*(2)Se 1 - N 4	/717. RY*(2) C 32	0.06	0.92	0.013

from unit 2 to unit 1

39. BD (1) N 27 - C 28	/788. BD*(1)Se 1 - N 4	0.16	1.10	0.012
40. BD (1) N 27 - C 29	/788. BD*(1)Se 1 - N 4	0.16	1.10	0.012
41. BD (2) N 27 - C 29	/432. RY*(2) H 17	0.06	2.84	0.013
41. BD (2) N 27 - C 29	/788. BD*(1)Se 1 - N 4	0.21	0.53	0.010
41. BD (2) N 27 - C 29	/817. BD*(1) C 16 - H 17	0.18	0.88	0.012
42. BD (1) C 28 - C 30	/788. BD*(1)Se 1 - N 4	0.14	0.97	0.011
45. BD (1) C 29 - C 32	/788. BD*(1)Se 1 - N 4	0.14	0.97	0.011
84. CR (1) N 27	/788. BD*(1)Se 1 - N 4	0.06	14.40	0.028
95. LP (1) N 27	/ 96. RY*(1)Se 1	0.74	1.74	0.033
95. LP (1) N 27	/ 98. RY*(3)Se 1	0.11	1.33	0.011
95. LP (1) N 27	/102. RY*(7)Se 1	0.10	1.94	0.013
95. LP (1) N 27	/409. RY*(5) C 16	0.06	2.24	0.011
95. LP (1) N 27	/788. BD*(1)Se 1 - N 4	11.72	0.60	0.076
95. LP (1) N 27	/790. BD*(1)Se 1 - C 9	0.57	0.66	0.018
95. LP (1) N 27	/797. BD*(1) C 5 - C 9	0.29	1.05	0.016
95. LP (1) N 27	/817. BD*(1) C 16 - H 17	0.34	0.95	0.016
95. LP (1) N 27	/818. BD*(1) C 16 - C 22	0.24	1.09	0.015
828. BD*(2) N 27 - C 29	/788. BD*(1)Se 1 - N 4	0.27	0.12	0.010
828. BD*(2) N 27 - C 29	/817. BD*(1) C 16 - H 17	0.09	0.46	0.013
830. BD*(2) C 28 - C 30	/819. BD*(2) C 16 - C 22	0.08	0.02	0.002

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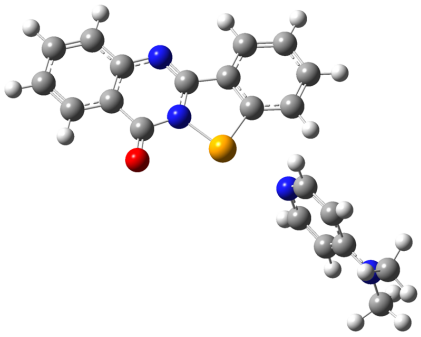
3.DMAP



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Sum of electronic and thermal Enthalpies= -3506.593296
Sum of electronic and thermal Free Energies= -3506.675816

1	Se			
2	C	4.0988951		
3	H	1.0822571	132.0093838	
4	N	1.8886157	62.9094797	0.0009172
5	C	1.3903154	13.3326133	0.0039338
6	C	1.3796235	106.0247001	-179.9983017
7	H	1.0821112	120.1512375	179.9989505
8	C	1.3825108	119.1980730	-179.9961648
9	C	1.3950636	120.7086696	0.0024707
10	C	2.4769239	142.0307291	179.9979300
11	H	1.0822573	87.5522965	179.9974192
12	N	2.3552384	143.8784042	-0.0048268
13	O	1.2163057	120.6032072	-0.0035947

14	C	2.3991950	120.3334356	-0.0027565
15	H	1.0831542	149.3974751	-179.9994123
16	C	1.3901002	119.8868446	0.0000000
17	H	1.0796856	120.3983882	179.9996477
18	C	1.3759124	88.0739587	-179.9942675
19	C	1.2905785	28.4323293	0.0053619
20	C	1.3735093	150.8052379	-0.0031887
21	H	1.0821609	120.2764902	-179.9994506
22	C	1.3834466	118.9508623	0.0000000
23	H	1.0830256	119.0987385	-179.9996577
24	C	1.3731639	91.0168921	0.0004297
25	H	1.0820314	121.5619537	180.0000000
26	C	1.3983083	30.6956910	-0.0017033
27	N	2.6709579	174.5207770	-0.0128247
28	C	1.3317985	120.4207654	-99.3053258
29	C	1.3317969	120.4332713	99.3129882
30	C	1.3767030	124.2100751	-162.3953014
31	H	1.0850302	115.9657699	17.4288037
32	C	1.3767040	124.2100083	162.3928137
33	H	1.0850292	115.9658863	-17.4321402
34	C	1.4074417	119.4581441	-0.1616757
35	H	1.0793185	118.8907101	179.8272549
36	H	1.0793185	118.8904974	-179.8292147
37	N	1.3589303	121.9802273	-179.9249766
38	C	1.4458887	120.0499415	1.1076371
39	H	1.0945336	111.7519423	60.7647772
40	H	1.0867652	109.2252517	-179.8143895
41	H	1.0940533	111.5713227	-60.6367885
42	C	1.4458868	120.0500830	178.8056517
43	H	1.0940497	111.5700023	60.6089225
44	H	1.0867662	109.2251882	179.7845635
45	H	1.0945373	111.7534664	-60.7928145

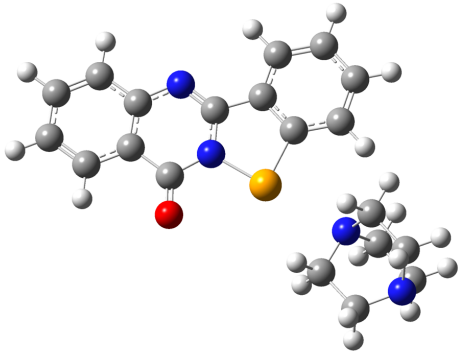
Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
1. BD (1)Se 1 - N 4	/622. RY*(1) N 27	0.61	1.89	0.031
1. BD (1)Se 1 - N 4	/624. RY*(3) N 27	0.11	1.50	0.011
2. BD (1)Se 1 - C 9	/622. RY*(1) N 27	0.27	1.86	0.020
16. BD (1) C 9 - C 16	/622. RY*(1) N 27	0.05	2.00	0.009
16. BD (1) C 9 - C 16	/624. RY*(3) N 27	0.07	1.61	0.010
28. BD (1) C 16 - H 17	/107. LP (2) N 27	0.51	0.38	0.020
60. CR (3)Se 1	/942. BD*(1) N 27 - C 28	0.07	11.39	0.025
60. CR (3)Se 1	/943. BD*(1) N 27 - C 29	0.07	11.39	0.025
98. LP (1)Se 1	/107. LP (2) N 27	0.46	0.57	0.024
98. LP (1)Se 1	/622. RY*(1) N 27	0.09	1.98	0.012
98. LP (1)Se 1	/942. BD*(1) N 27 - C 28	0.61	1.39	0.026
98. LP (1)Se 1	/943. BD*(1) N 27 - C 29	0.61	1.39	0.026
99. LP (2)Se 1	/649. RY*(2) C 28	0.05	1.71	0.009
99. LP (2)Se 1	/675. RY*(2) C 29	0.05	1.71	0.009
99. LP (2)Se 1	/942. BD*(1) N 27 - C 28	0.24	0.89	0.014
99. LP (2)Se 1	/943. BD*(1) N 27 - C 29	0.24	0.89	0.014
99. LP (2)Se 1	/944. BD*(1) C 28 - C 30	0.10	0.93	0.009
99. LP (2)Se 1	/947. BD*(1) C 29 - C 32	0.10	0.93	0.009
from unit 2 to unit 1				

37. BD (1) N 27 - C 28	/906. BD*(1)Se 1 - N 4	0.24	1.08	0.015
38. BD (1) N 27 - C 29	/906. BD*(1)Se 1 - N 4	0.24	1.08	0.015
39. BD (1) C 28 - C 30	/906. BD*(1)Se 1 - N 4	0.17	0.97	0.012
42. BD (1) C 29 - C 32	/906. BD*(1)Se 1 - N 4	0.17	0.97	0.012
89. CR (1) N 27	/906. BD*(1)Se 1 - N 4	0.11	14.39	0.036
106. LP (1) N 27	/110. RY*(1)Se 1	1.06	1.70	0.039
106. LP (1) N 27	/113. RY*(4)Se 1	0.07	1.37	0.009
106. LP (1) N 27	/116. RY*(7)Se 1	0.15	1.91	0.016
106. LP (1) N 27	/171. RY*(1) N 4	0.07	1.70	0.010
106. LP (1) N 27	/424. RY*(5) C 16	0.09	2.24	0.013
106. LP (1) N 27	/446. RY*(1) H 17	0.06	1.30	0.008
106. LP (1) N 27	/447. RY*(2) H 17	0.06	2.92	0.012
106. LP (1) N 27	/906. BD*(1)Se 1 - N 4	16.23	0.60	0.089
106. LP (1) N 27	/907. BD*(1)Se 1 - C 9	0.90	0.65	0.022
106. LP (1) N 27	/914. BD*(1) C 5 - C 9	0.36	1.05	0.018
106. LP (1) N 27	/933. BD*(1) C 16 - H 17	0.32	0.95	0.016
106. LP (1) N 27	/934. BD*(1) C 16 - C 22	0.27	1.09	0.016
107. LP (2) N 27	/119. RY*(10)Se 1	0.06	2.44	0.014
107. LP (2) N 27	/906. BD*(1)Se 1 - N 4	0.63	0.38	0.016
107. LP (2) N 27	/933. BD*(1) C 16 - H 17	0.44	0.73	0.020
107. LP (2) N 27	/934. BD*(1) C 16 - C 22	0.08	0.87	0.009
945. BD*(2) C 28 - C 30	/935. BD*(2) C 16 - C 22	0.12	0.02	0.002
948. BD*(2) C 29 - C 32	/935. BD*(2) C 16 - C 22	0.12	0.02	0.002

3.DABCO



Sum of electronic and zero-point Energies= -3469.679848
Sum of electronic and thermal Energies= -3469.658725
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1	Se			
2	C	4.0932446		
3	H	1.0822458	132.2439593	
4	N	1.8794178	63.1590402	0.1182993
5	C	1.3900384	13.4846917	0.0614651
6	C	1.3800925	105.8503125	-179.8836063
7	H	1.0819517	120.1117509	-179.9926896
8	C	1.3825573	118.9508715	-179.8084309
9	C	1.3943430	120.5750374	-0.0409846
10	C	2.4760273	141.9345246	179.8301809
11	H	1.0821996	87.6118868	179.9420377
12	N	2.3530665	143.9676194	-0.2945650
13	O	1.2163530	120.4117697	-0.1729064
14	C	2.3993231	120.3024151	-0.0676704
15	H	1.0830553	149.3827632	-179.9816182
16	C	1.3883744	120.0563014	-0.0673819
17	H	1.0791317	120.6247502	-179.8668638
18	C	1.3768822	87.9877794	-179.6860699

19	C	1.2890526	28.5908040	0.2799689
20	C	1.3734401	150.7603532	-0.0824127
21	H	1.0820855	120.2582180	-179.9713195
22	C	1.3832806	118.9925804	0.0659712
23	H	1.0828681	119.2475927	-179.9907044
24	C	1.3733016	91.0384875	0.0125731
25	H	1.0819610	121.5596005	-179.9908094
26	C	1.3983032	30.6874715	-0.0378243
27	C	3.2102700	152.3722489	178.3711084
28	C	2.3864880	80.6427329	-146.3131208
29	C	2.3856672	82.4901728	152.7586659
30	C	1.5522755	169.9301789	-166.0138786
31	H	1.0915815	71.9782612	-53.3519730
32	H	1.0915620	75.0226046	60.9124951
33	H	1.0916048	144.1778233	-48.5028190
34	H	1.0912871	89.6981792	71.6426503
35	C	1.5541576	89.8024400	-176.4659480
36	C	1.5545647	89.7756255	173.3147628
37	H	1.0915760	144.2729276	45.5344590
38	H	1.0912488	89.7387716	-74.7914684
39	H	1.0913510	111.1903218	109.4225511
40	H	1.0913557	111.2005528	-130.8594872
41	H	1.0916247	111.1876296	150.0336050
42	H	1.0914111	111.1875177	-90.2446733
43	H	1.0916227	111.1745824	-150.1369449
44	H	1.0914245	111.1803025	90.1482321
45	N	1.4661715	35.6624677	47.6659965
46	N	1.4595220	110.0849545	-29.9906425

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

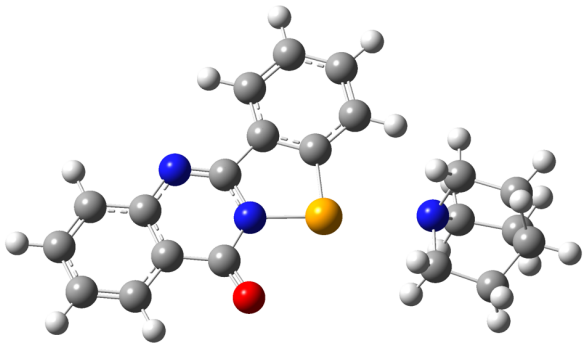
Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
1. BD (1)Se 1 - N 4	/833. RY*(1) N 45	0.54	1.77	0.028
1. BD (1)Se 1 - N 4	/834. RY*(2) N 45	0.06	2.39	0.011
2. BD (2)Se 1 - N 4	/835. RY*(3) N 45	0.14	1.68	0.015
2. BD (2)Se 1 - N 4	/848. RY*(16) N 45	0.06	4.06	0.015
3. BD (1)Se 1 - C 9	/833. RY*(1) N 45	0.24	1.73	0.018
30. BD (1) C 16 - H 17	/926. BD*(1) C 27 - N 45	0.14	1.02	0.011
30. BD (1) C 16 - H 17	/927. BD*(1) C 28 - H 33	0.07	1.06	0.008
30. BD (1) C 16 - H 17	/929. BD*(1) C 28 - C 35	0.06	1.01	0.007
30. BD (1) C 16 - H 17	/931. BD*(1) C 29 - C 36	0.06	1.01	0.007
30. BD (1) C 16 - H 17	/932. BD*(1) C 29 - H 37	0.09	1.06	0.009
99. LP (1)Se 1	/923. BD*(1) C 27 - C 30	0.80	1.20	0.028
99. LP (1)Se 1	/930. BD*(1) C 28 - N 45	0.43	1.20	0.020
99. LP (1)Se 1	/934. BD*(1) C 29 - N 45	0.54	1.20	0.023
100. LP (2)Se 1	/625. RY*(9) C 27	0.11	1.30	0.013
100. LP (2)Se 1	/644. RY*(2) C 28	0.12	1.48	0.015
100. LP (2)Se 1	/645. RY*(3) C 28	0.32	1.37	0.023
100. LP (2)Se 1	/648. RY*(6) C 28	0.05	2.16	0.011
100. LP (2)Se 1	/651. RY*(9) C 28	0.07	1.71	0.012
100. LP (2)Se 1	/658. RY*(16) C 28	0.08	3.16	0.017
100. LP (2)Se 1	/659. RY*(17) C 28	0.09	20.42	0.046
100. LP (2)Se 1	/670. RY*(2) C 29	0.09	1.48	0.012
100. LP (2)Se 1	/671. RY*(3) C 29	0.22	1.37	0.019
100. LP (2)Se 1	/672. RY*(4) C 29	0.06	2.07	0.012
100. LP (2)Se 1	/677. RY*(9) C 29	0.07	1.68	0.012

100. LP (2)Se 1 /687. RY*(19) C 29 0.10 20.34 0.049
100. LP (2)Se 1 /721. RY*(1) H 31 0.30 1.13 0.020
100. LP (2)Se 1 /726. RY*(1) H 32 0.27 1.11 0.019
100. LP (2)Se 1 /736. RY*(1) H 34 0.06 1.02 0.009
100. LP (2)Se 1 /745. RY*(5) C 35 0.05 2.24 0.012
100. LP (2)Se 1 /834. RY*(2) N 45 0.07 1.65 0.011
100. LP (2)Se 1 /835. RY*(3) N 45 2.04 1.33 0.056
100. LP (2)Se 1 /837. RY*(5) N 45 0.06 2.91 0.014
100. LP (2)Se 1 /841. RY*(9) N 45 0.29 4.21 0.038
100. LP (2)Se 1 /848. RY*(16) N 45 0.91 3.71 0.063
100. LP (2)Se 1 /924. BD*(1) C 27 - H 31 0.25 0.43 0.011
100. LP (2)Se 1 /925. BD*(1) C 27 - H 32 0.18 0.43 0.009
100. LP (2)Se 1 /928. BD*(1) C 28 - H 34 0.06 0.43 0.005
100. LP (2)Se 1 /929. BD*(1) C 28 - C 35 0.14 0.38 0.008
100. LP (2)Se 1 /930. BD*(1) C 28 - N 45 0.11 0.39 0.007
100. LP (2)Se 1 /931. BD*(1) C 29 - C 36 0.09 0.38 0.006
100. LP (2)Se 1 /934. BD*(1) C 29 - N 45 0.13 0.39 0.008
886. BD*(2)Se 1 - N 4 /625. RY*(9) C 27 0.28 0.69 0.026
886. BD*(2)Se 1 - N 4 /644. RY*(2) C 28 0.11 0.86 0.018
886. BD*(2)Se 1 - N 4 /645. RY*(3) C 28 0.30 0.75 0.028
886. BD*(2)Se 1 - N 4 /646. RY*(4) C 28 0.05 1.48 0.016
886. BD*(2)Se 1 - N 4 /648. RY*(6) C 28 0.11 1.55 0.024
886. BD*(2)Se 1 - N 4 /651. RY*(9) C 28 0.10 1.10 0.020
886. BD*(2)Se 1 - N 4 /658. RY*(16) C 28 0.11 2.55 0.032
886. BD*(2)Se 1 - N 4 /659. RY*(17) C 28 0.09 19.80 0.079
886. BD*(2)Se 1 - N 4 /670. RY*(2) C 29 0.08 0.86 0.015
886. BD*(2)Se 1 - N 4 /671. RY*(3) C 29 0.18 0.75 0.022
886. BD*(2)Se 1 - N 4 /672. RY*(4) C 29 0.10 1.45 0.022
886. BD*(2)Se 1 - N 4 /674. RY*(6) C 29 0.08 1.62 0.021
886. BD*(2)Se 1 - N 4 /677. RY*(9) C 29 0.09 1.07 0.018
886. BD*(2)Se 1 - N 4 /687. RY*(19) C 29 0.11 19.72 0.084
886. BD*(2)Se 1 - N 4 /721. RY*(1) H 31 0.45 0.51 0.028
886. BD*(2)Se 1 - N 4 /726. RY*(1) H 32 0.40 0.50 0.026
886. BD*(2)Se 1 - N 4 /736. RY*(1) H 34 0.05 0.40 0.009
886. BD*(2)Se 1 - N 4 /745. RY*(5) C 35 0.06 1.62 0.018
886. BD*(2)Se 1 - N 4 /818. RY*(1) H 42 0.06 0.42 0.010
886. BD*(2)Se 1 - N 4 /828. RY*(1) H 44 0.06 0.42 0.009
886. BD*(2)Se 1 - N 4 /834. RY*(2) N 45 0.09 1.04 0.018
886. BD*(2)Se 1 - N 4 /835. RY*(3) N 45 2.87 0.72 0.084
886. BD*(2)Se 1 - N 4 /841. RY*(9) N 45 0.30 3.60 0.060
886. BD*(2)Se 1 - N 4 /848. RY*(16) N 45 1.14 3.10 0.110
886. BD*(2)Se 1 - N 4 /855. RY*(23) N 45 0.08 3.59 0.031

from unit 2 to unit 1
40. BD (1) C 27 - H 31 /111. RY*(6)Se 1 0.06 1.97 0.010
40. BD (1) C 27 - H 31 /885. BD*(1)Se 1 - N 4 0.10 0.73 0.008
40. BD (1) C 27 - H 31 /887. BD*(1)Se 1 - C 9 0.14 0.79 0.009
41. BD (1) C 27 - H 32 /111. RY*(6)Se 1 0.08 1.97 0.011
41. BD (1) C 27 - H 32 /885. BD*(1)Se 1 - N 4 0.08 0.73 0.007
41. BD (1) C 27 - H 32 /887. BD*(1)Se 1 - C 9 0.10 0.79 0.008
42. BD (1) C 27 - N 45 /885. BD*(1)Se 1 - N 4 0.16 0.94 0.011
43. BD (1) C 28 - H 33 /441. RY*(1) H 17 0.20 1.57 0.016
43. BD (1) C 28 - H 33 /914. BD*(1) C 16 - H 17 0.24 1.08 0.014
44. BD (1) C 28 - H 34 /111. RY*(6)Se 1 0.11 1.97 0.013
45. BD (1) C 28 - C 35 /885. BD*(1)Se 1 - N 4 0.10 0.83 0.008
46. BD (1) C 28 - N 45 /885. BD*(1)Se 1 - N 4 0.09 0.94 0.008
46. BD (1) C 28 - N 45 /914. BD*(1) C 16 - H 17 0.05 1.29 0.007
47. BD (1) C 29 - C 36 /885. BD*(1)Se 1 - N 4 0.11 0.83 0.009
48. BD (1) C 29 - H 37 /441. RY*(1) H 17 0.25 1.57 0.018
48. BD (1) C 29 - H 37 /914. BD*(1) C 16 - H 17 0.34 1.08 0.017
49. BD (1) C 29 - H 38 /111. RY*(6)Se 1 0.05 1.97 0.009

50. BD (1) C 29 - N 45	/885. BD*(1)Se 1 - N 4	0.08	0.94	0.008
50. BD (1) C 29 - N 45	/914. BD*(1) C 16 - H 17	0.06	1.29	0.008
97. CR (1) N 45	/885. BD*(1)Se 1 - N 4	0.06	14.42	0.026
104. LP (1) N 45	/106. RY*(1)Se 1	0.84	1.55	0.033
104. LP (1) N 45	/108. RY*(3)Se 1	0.19	1.35	0.015
104. LP (1) N 45	/113. RY*(8)Se 1	0.06	2.20	0.010
104. LP (1) N 45	/116. RY*(11)Se 1	0.08	2.08	0.012
104. LP (1) N 45	/275. RY*(1) C 9	0.05	1.69	0.009
104. LP (1) N 45	/885. BD*(1)Se 1 - N 4	10.39	0.54	0.068
104. LP (1) N 45	/887. BD*(1)Se 1 - C 9	0.70	0.60	0.019
104. LP (1) N 45	/894. BD*(1) C 5 - C 9	0.14	0.99	0.011
104. LP (1) N 45	/915. BD*(1) C 16 - C 22	0.07	1.03	0.008

3.quinuclidine



Sum of electronic and zero-point Energies= -3453.649486
Sum of electronic and thermal Energies= -3453.628160
Sum of electronic and thermal Enthalpies= -3453.627216
Sum of electronic and thermal Free Energies= -3453.703126

1	Se			
2	C	4.0942624		
3	H	1.0822505	132.2309103	
4	N	1.8817210	63.1100182	-0.0690438
5	C	1.3900537	13.4873151	-0.0158606
6	C	1.3800523	105.8578719	179.9366282
7	H	1.0819672	120.1226171	179.9922656
8	C	1.3824740	118.9840238	179.9627395
9	C	1.3944558	120.5978022	0.0421794
10	C	2.4762285	141.9491909	179.9677112
11	H	1.0822081	87.6005105	-179.9395081
12	N	2.3535102	143.9608441	0.0684630
13	O	1.2163973	120.4505540	0.0076146
14	C	2.3993082	120.3092525	0.0558576
15	H	1.0830729	149.3865527	-179.9907300
16	C	1.3884127	120.0075791	0.0488852
17	H	1.0789642	120.6272836	179.8667197
18	C	1.3766919	88.0004608	179.9771539
19	C	1.2893375	28.5567071	-0.0295614
20	C	1.3734518	150.7695978	0.0491041
21	H	1.0820982	120.2616590	-179.9878506
22	C	1.3832579	119.0243089	-0.0488513
23	H	1.0828857	119.2358600	179.9903955
24	C	1.3732721	91.0335438	0.0065269
25	H	1.0819752	121.5602207	-179.9990747
26	C	1.3983061	30.6880168	0.0631682
27	C	3.2010895	152.2892376	178.6405585

28	C	2.3904863	81.6611740	-150.5956194
29	C	2.3911800	80.6498604	148.3704996
30	C	1.5471353	169.9952631	145.1830800
31	H	1.0913608	77.5900979	-61.8983066
32	H	1.0914088	68.9462593	51.9787765
33	H	1.0913882	143.4255918	-53.7385043
34	H	1.0909755	92.4287578	69.6619084
35	C	1.5488453	89.2853468	-178.7499831
36	C	1.5488193	93.8043276	172.5837293
37	H	1.0912234	143.6350290	38.4020622
38	H	1.0911288	86.7827896	-76.1498345
39	C	1.5304281	108.0198118	39.6323658
40	H	1.0914053	110.6469557	160.5542493
41	H	1.0920524	110.8240549	-80.7731807
42	H	1.0916372	110.6870740	157.3024265
43	H	1.0920673	110.8211941	-83.9863851
44	H	1.0923404	110.8378178	-143.8301098
45	H	1.0914816	110.6866858	97.4653883
46	H	1.0904053	110.3497572	175.4315766
47	N	1.4662761	35.4684864	50.3461613

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

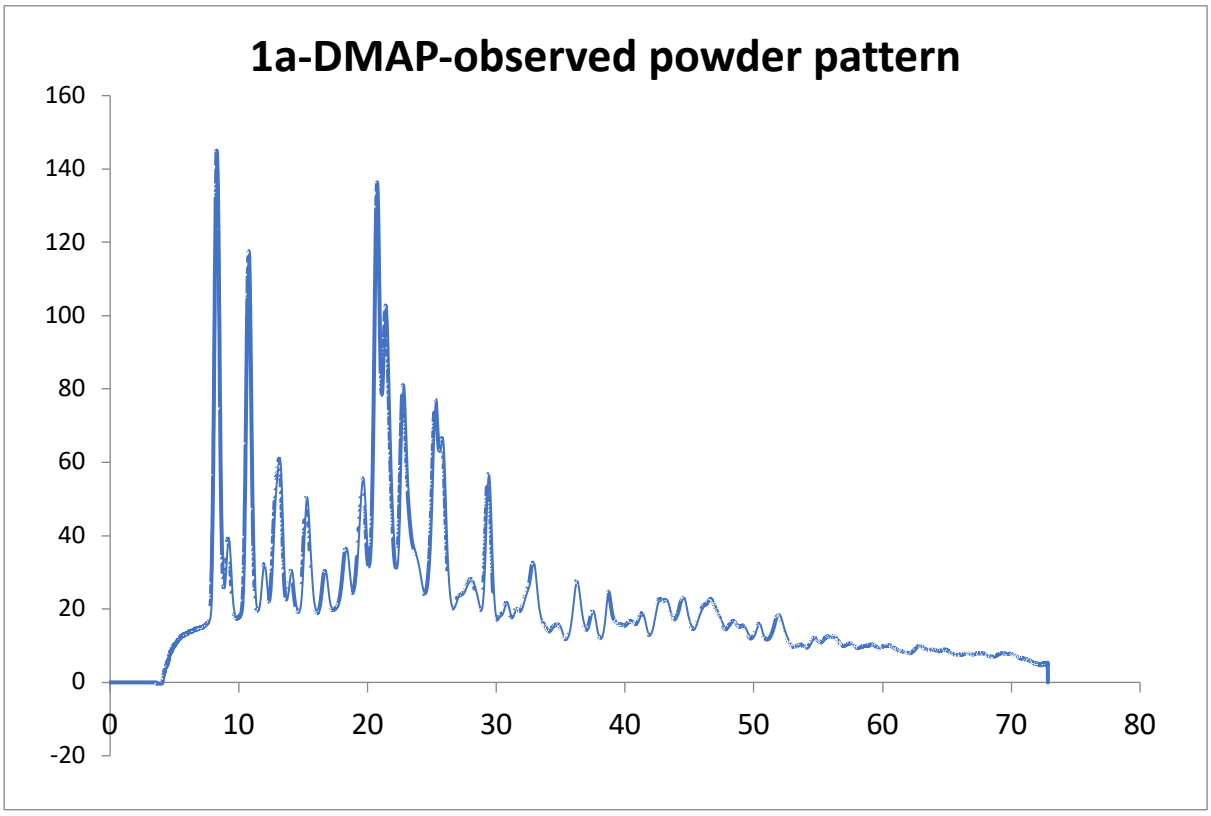
(Intermolecular threshold: 0.05 kcal/mol)

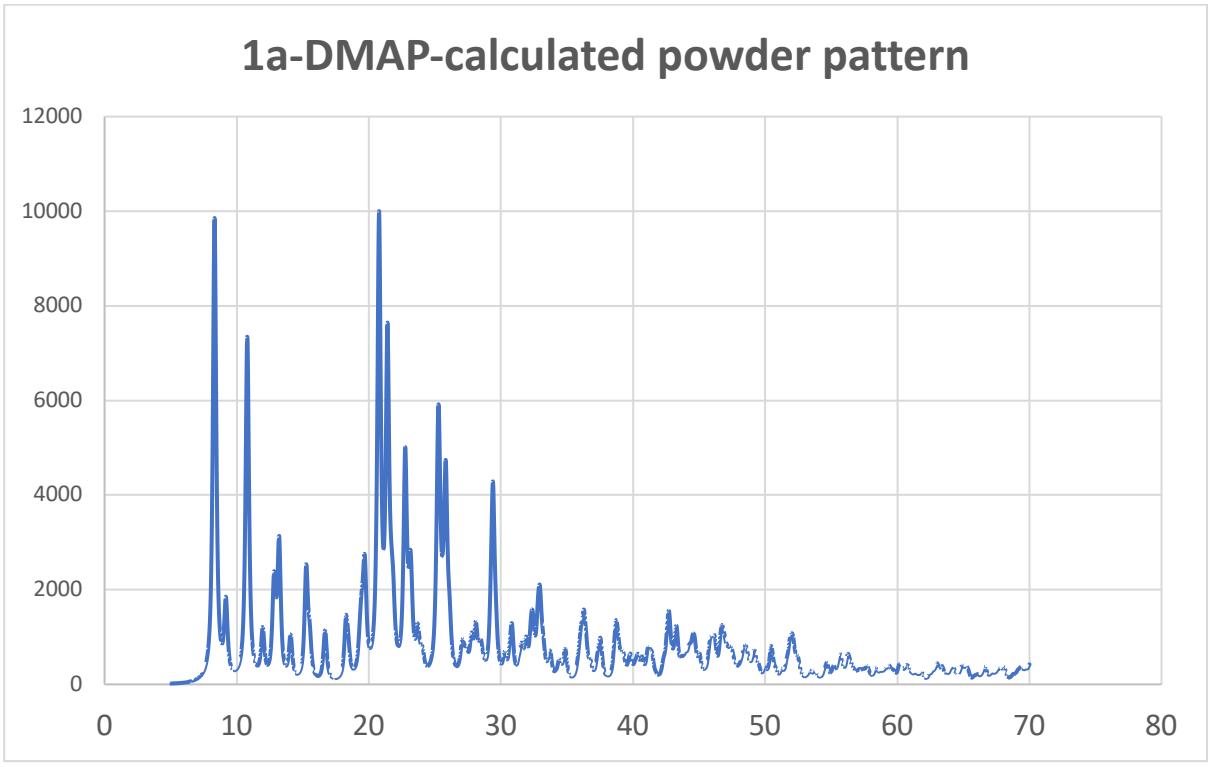
Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
from unit 1 to unit 2				
1. BD (1)Se 1 - N 4	/864. RY*(1) N 47	0.57	1.77	0.028
1. BD (1)Se 1 - N 4	/865. RY*(2) N 47	0.06	2.51	0.011
2. BD (2)Se 1 - N 4	/866. RY*(3) N 47	0.13	1.71	0.015
2. BD (2)Se 1 - N 4	/879. RY*(16) N 47	0.06	4.05	0.015
3. BD (1)Se 1 - C 9	/627. RY*(11) C 27	0.06	2.86	0.012
3. BD (1)Se 1 - C 9	/864. RY*(1) N 47	0.25	1.73	0.019
30. BD (1) C 16 - H 17	/931. BD*(1) C 27 - N 47	0.13	1.03	0.010
30. BD (1) C 16 - H 17	/932. BD*(1) C 28 - H 33	0.08	1.06	0.008
30. BD (1) C 16 - H 17	/934. BD*(1) C 28 - C 35	0.09	1.02	0.009
30. BD (1) C 16 - H 17	/937. BD*(1) C 29 - H 37	0.08	1.06	0.008
100. LP (1)Se 1	/928. BD*(1) C 27 - C 30	0.83	1.21	0.028
100. LP (1)Se 1	/935. BD*(1) C 28 - N 47	0.53	1.21	0.023
100. LP (1)Se 1	/939. BD*(1) C 29 - N 47	0.45	1.21	0.021
101. LP (2)Se 1	/625. RY*(9) C 27	0.11	1.28	0.013
101. LP (2)Se 1	/645. RY*(3) C 28	0.29	1.34	0.021
101. LP (2)Se 1	/651. RY*(9) C 28	0.06	1.53	0.010
101. LP (2)Se 1	/658. RY*(16) C 28	0.06	2.44	0.013
101. LP (2)Se 1	/659. RY*(17) C 28	0.09	20.47	0.047
101. LP (2)Se 1	/670. RY*(2) C 29	0.07	1.46	0.011
101. LP (2)Se 1	/671. RY*(3) C 29	0.39	1.32	0.025
101. LP (2)Se 1	/674. RY*(6) C 29	0.11	2.29	0.017
101. LP (2)Se 1	/676. RY*(8) C 29	0.05	1.72	0.010
101. LP (2)Se 1	/677. RY*(9) C 29	0.05	1.33	0.009
101. LP (2)Se 1	/684. RY*(16) C 29	0.06	2.61	0.013
101. LP (2)Se 1	/687. RY*(19) C 29	0.09	20.56	0.045
101. LP (2)Se 1	/721. RY*(1) H 31	0.25	1.18	0.019
101. LP (2)Se 1	/726. RY*(1) H 32	0.29	1.19	0.020
101. LP (2)Se 1	/747. RY*(7) C 35	0.05	2.01	0.011
101. LP (2)Se 1	/773. RY*(7) C 36	0.09	2.17	0.015
101. LP (2)Se 1	/866. RY*(3) N 47	1.87	1.36	0.054
101. LP (2)Se 1	/868. RY*(5) N 47	0.05	2.82	0.013
101. LP (2)Se 1	/872. RY*(9) N 47	0.26	4.10	0.035
101. LP (2)Se 1	/879. RY*(16) N 47	0.88	3.70	0.062

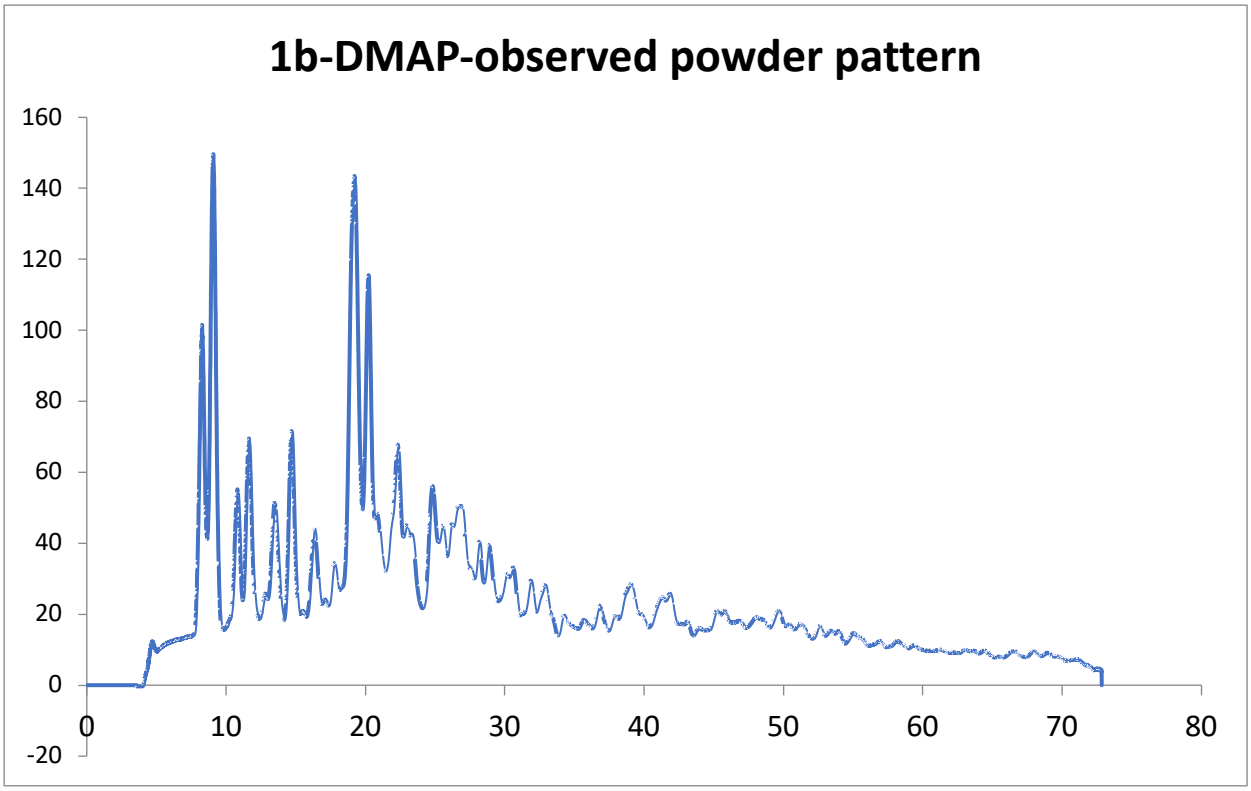
101. LP (2)Se 1	/929. BD*(1) C 27 - H 31	0.11	0.43	0.007
101. LP (2)Se 1	/930. BD*(1) C 27 - H 32	0.32	0.44	0.013
101. LP (2)Se 1	/934. BD*(1) C 28 - C 35	0.10	0.39	0.007
101. LP (2)Se 1	/935. BD*(1) C 28 - N 47	0.12	0.39	0.007
101. LP (2)Se 1	/936. BD*(1) C 29 - C 36	0.14	0.39	0.008
101. LP (2)Se 1	/939. BD*(1) C 29 - N 47	0.13	0.39	0.008
891. BD*(2)Se 1 - N 4	/625. RY*(9) C 27	0.29	0.67	0.026
891. BD*(2)Se 1 - N 4	/645. RY*(3) C 28	0.25	0.72	0.025
891. BD*(2)Se 1 - N 4	/646. RY*(4) C 28	0.05	2.07	0.019
891. BD*(2)Se 1 - N 4	/647. RY*(5) C 28	0.08	1.44	0.020
891. BD*(2)Se 1 - N 4	/651. RY*(9) C 28	0.11	0.91	0.019
891. BD*(2)Se 1 - N 4	/658. RY*(16) C 28	0.12	1.83	0.027
891. BD*(2)Se 1 - N 4	/659. RY*(17) C 28	0.10	19.86	0.081
891. BD*(2)Se 1 - N 4	/670. RY*(2) C 29	0.06	0.85	0.013
891. BD*(2)Se 1 - N 4	/671. RY*(3) C 29	0.37	0.71	0.030
891. BD*(2)Se 1 - N 4	/674. RY*(6) C 29	0.18	1.68	0.032
891. BD*(2)Se 1 - N 4	/676. RY*(8) C 29	0.05	1.10	0.014
891. BD*(2)Se 1 - N 4	/677. RY*(9) C 29	0.11	0.72	0.017
891. BD*(2)Se 1 - N 4	/681. RY*(13) C 29	0.07	1.69	0.019
891. BD*(2)Se 1 - N 4	/684. RY*(16) C 29	0.07	2.00	0.022
891. BD*(2)Se 1 - N 4	/687. RY*(19) C 29	0.09	19.95	0.078
891. BD*(2)Se 1 - N 4	/721. RY*(1) H 31	0.34	0.57	0.026
891. BD*(2)Se 1 - N 4	/726. RY*(1) H 32	0.45	0.58	0.030
891. BD*(2)Se 1 - N 4	/773. RY*(7) C 36	0.07	1.56	0.019
891. BD*(2)Se 1 - N 4	/844. RY*(1) H 43	0.06	0.52	0.010
891. BD*(2)Se 1 - N 4	/866. RY*(3) N 47	2.66	0.74	0.082
891. BD*(2)Se 1 - N 4	/872. RY*(9) N 47	0.25	3.49	0.055
891. BD*(2)Se 1 - N 4	/875. RY*(12) N 47	0.05	2.15	0.020
891. BD*(2)Se 1 - N 4	/879. RY*(16) N 47	1.14	3.08	0.109

from unit 2 to unit 1

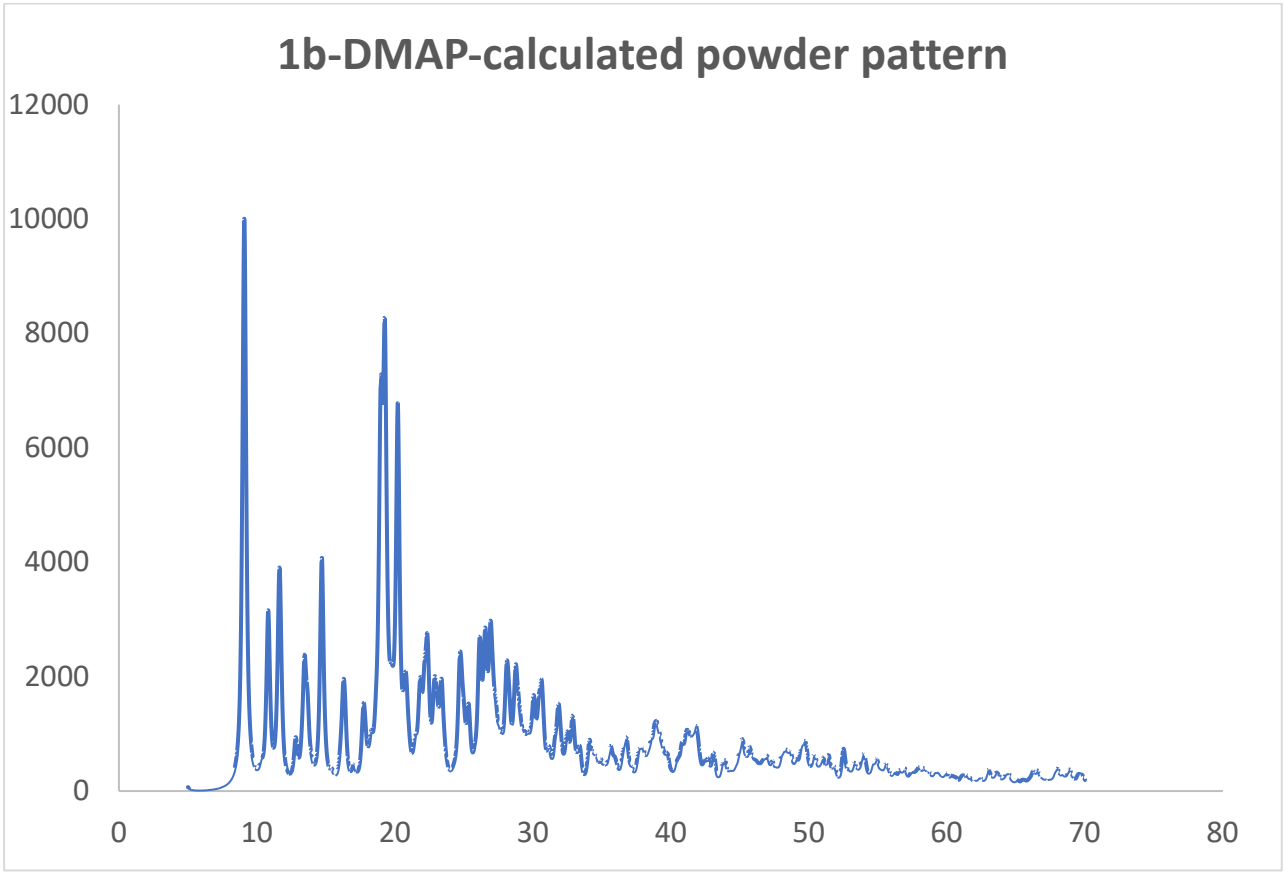
40. BD (1) C 27 - H 31	/111. RY*(6)Se 1	0.08	1.97	0.011
40. BD (1) C 27 - H 31	/890. BD*(1)Se 1 - N 4	0.07	0.73	0.006
40. BD (1) C 27 - H 31	/892. BD*(1)Se 1 - C 9	0.07	0.79	0.007
41. BD (1) C 27 - H 32	/108. RY*(3)Se 1	0.05	1.56	0.008
41. BD (1) C 27 - H 32	/111. RY*(6)Se 1	0.06	1.97	0.010
41. BD (1) C 27 - H 32	/890. BD*(1)Se 1 - N 4	0.12	0.73	0.008
41. BD (1) C 27 - H 32	/892. BD*(1)Se 1 - C 9	0.20	0.79	0.011
42. BD (1) C 27 - N 47	/890. BD*(1)Se 1 - N 4	0.17	0.94	0.011
43. BD (1) C 28 - H 33	/441. RY*(1) H 17	0.26	1.57	0.018
43. BD (1) C 28 - H 33	/919. BD*(1) C 16 - H 17	0.38	1.08	0.018
44. BD (1) C 28 - H 34	/111. RY*(6)Se 1	0.12	1.97	0.014
45. BD (1) C 28 - C 35	/890. BD*(1)Se 1 - N 4	0.10	0.83	0.008
46. BD (1) C 28 - N 47	/890. BD*(1)Se 1 - N 4	0.09	0.94	0.008
46. BD (1) C 28 - N 47	/919. BD*(1) C 16 - H 17	0.07	1.29	0.008
47. BD (1) C 29 - C 36	/890. BD*(1)Se 1 - N 4	0.10	0.83	0.008
48. BD (1) C 29 - H 37	/441. RY*(1) H 17	0.21	1.57	0.016
48. BD (1) C 29 - H 37	/919. BD*(1) C 16 - H 17	0.24	1.08	0.014
49. BD (1) C 29 - H 38	/112. RY*(7)Se 1	0.07	2.13	0.011
50. BD (1) C 29 - N 47	/890. BD*(1)Se 1 - N 4	0.09	0.94	0.008
50. BD (1) C 29 - N 47	/919. BD*(1) C 16 - H 17	0.05	1.29	0.007
99. CR (1) N 47	/890. BD*(1)Se 1 - N 4	0.06	14.41	0.027
105. LP (1) N 47	/106. RY*(1)Se 1	0.87	1.56	0.034
105. LP (1) N 47	/108. RY*(3)Se 1	0.17	1.36	0.014
105. LP (1) N 47	/110. RY*(5)Se 1	0.06	2.06	0.010
105. LP (1) N 47	/116. RY*(11)Se 1	0.08	2.11	0.012
105. LP (1) N 47	/275. RY*(1) C 9	0.05	1.68	0.009
105. LP (1) N 47	/890. BD*(1)Se 1 - N 4	11.07	0.53	0.070
105. LP (1) N 47	/892. BD*(1)Se 1 - C 9	0.75	0.59	0.019
105. LP (1) N 47	/899. BD*(1) C 5 - C 9	0.14	0.98	0.011
105. LP (1) N 47	/920. BD*(1) C 16 - C 22	0.07	1.02	0.008

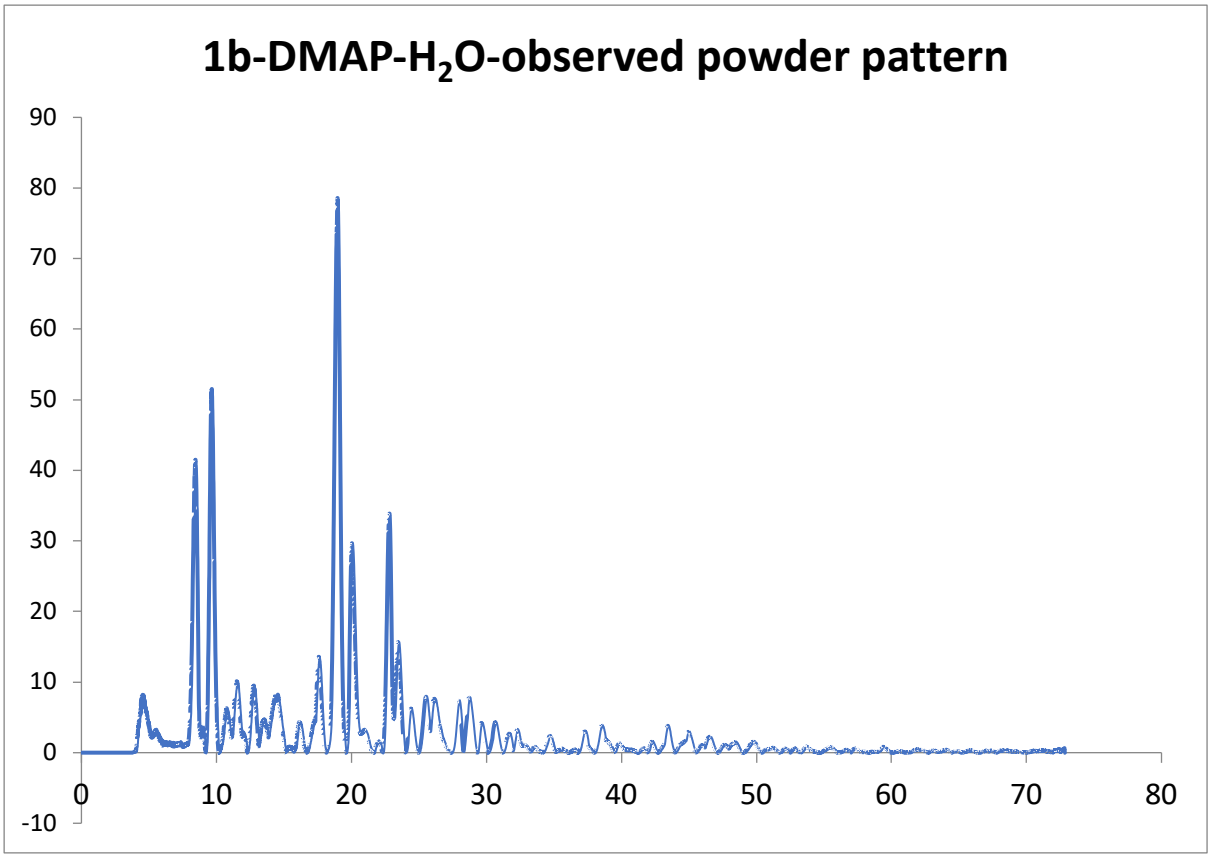

1a-DMAP-observed powder pattern
160
140
120
100
80
60
40
20
0
-20
0
10
20
30
40
50
60
70
80

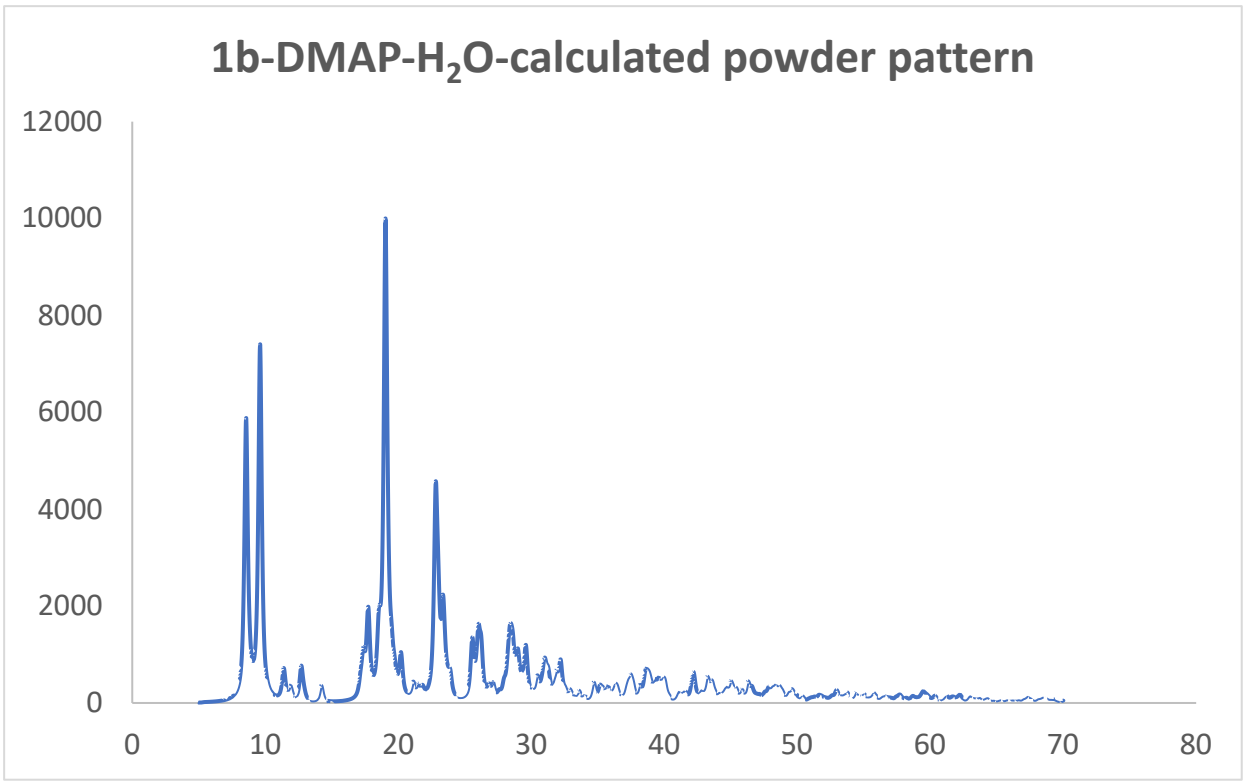

1a-DMAP-calculated powder pattern
12000
10000
8000
6000
4000
2000
0
0
10
20
30
40
50
60
70
80

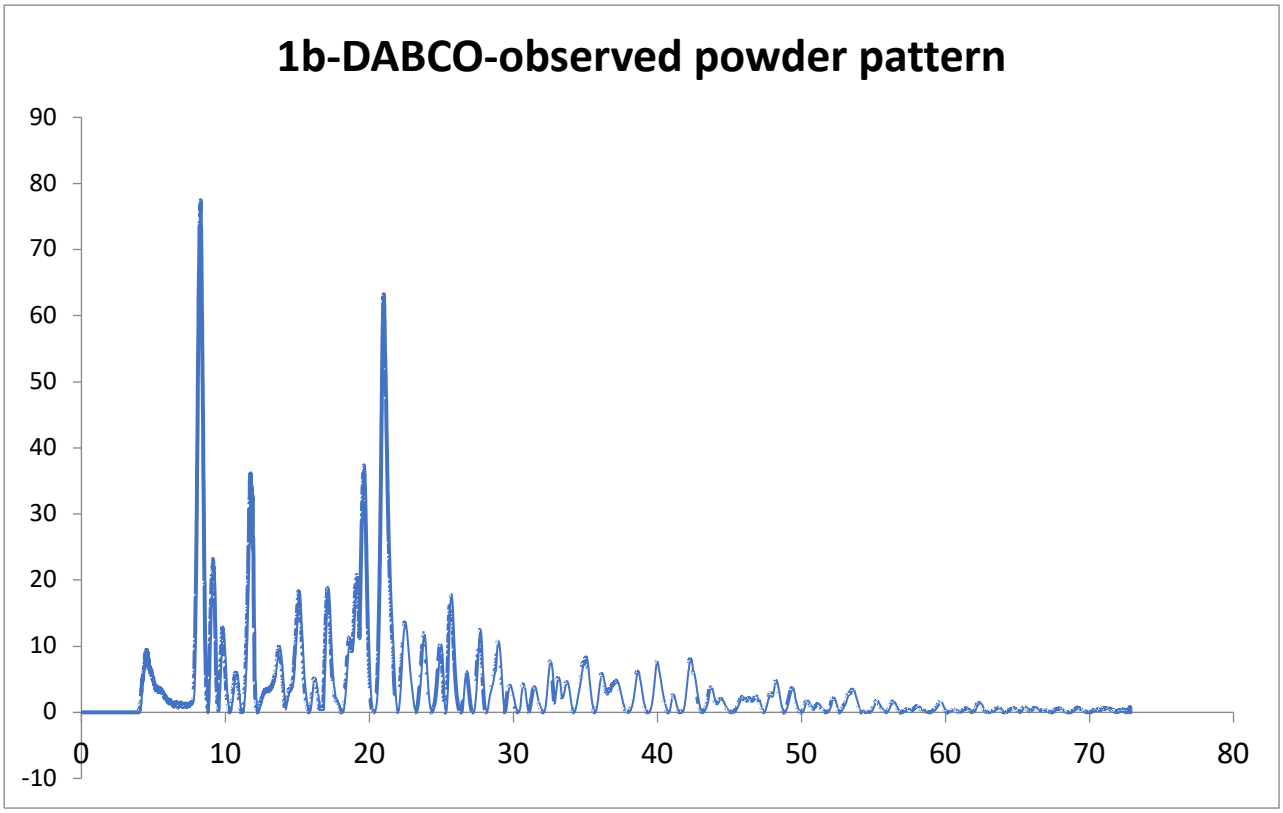


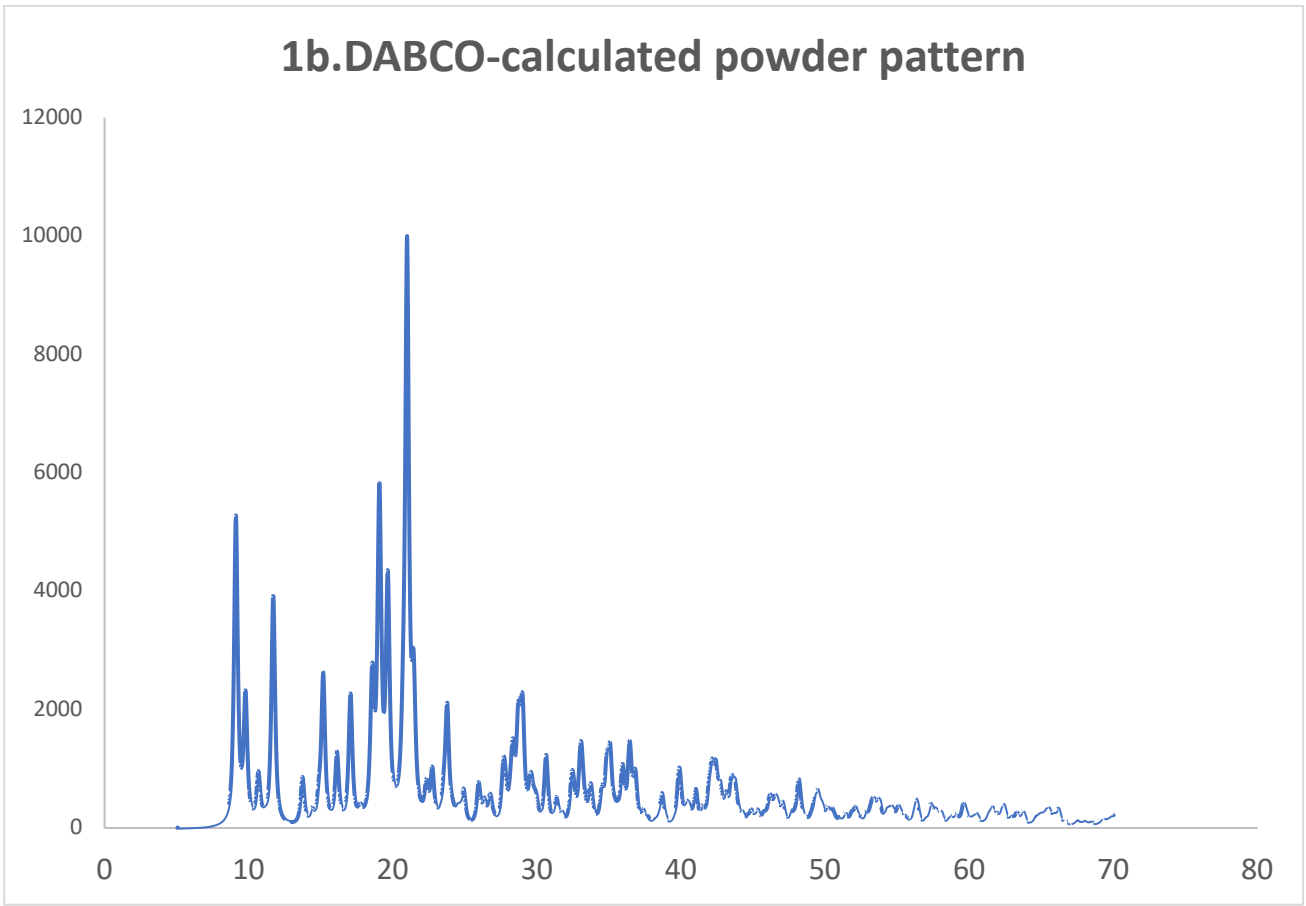
*Peak at ca. 8.5° is from ca. 30% of 1b

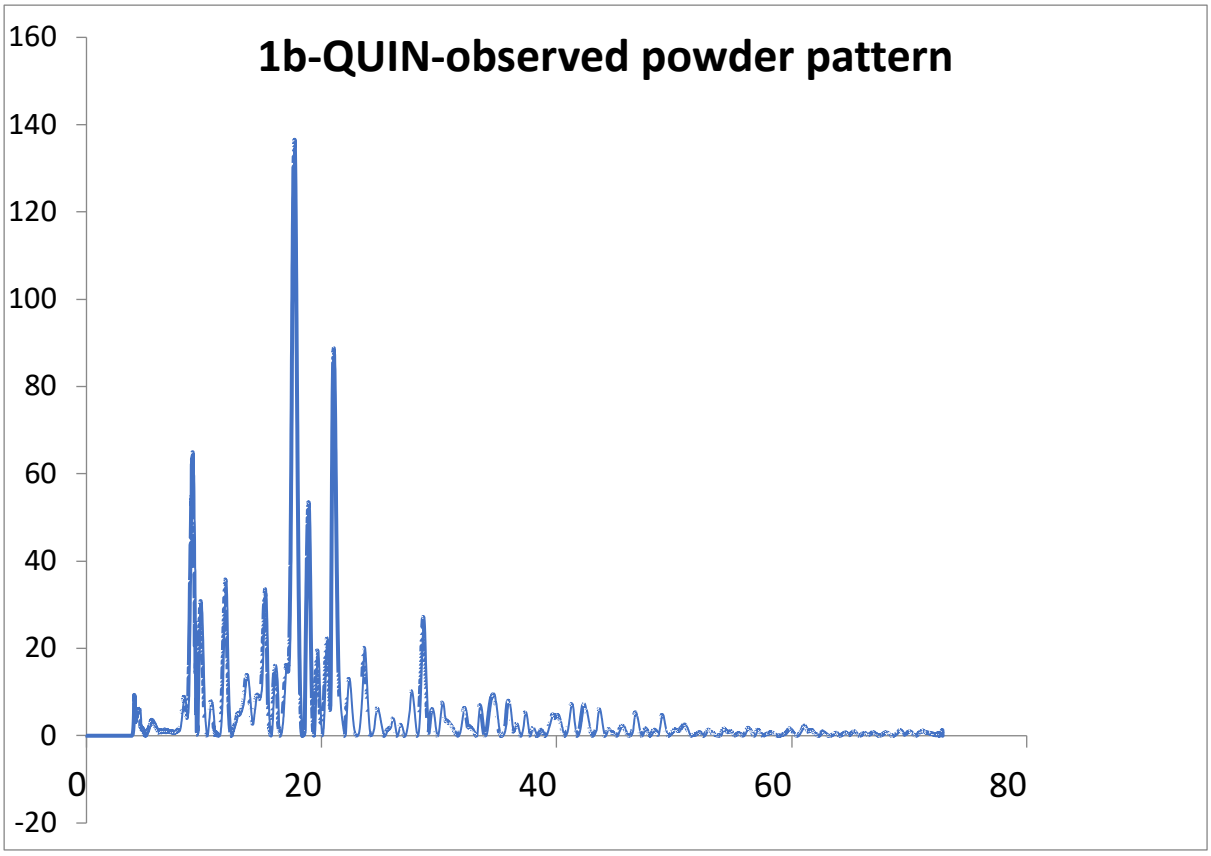


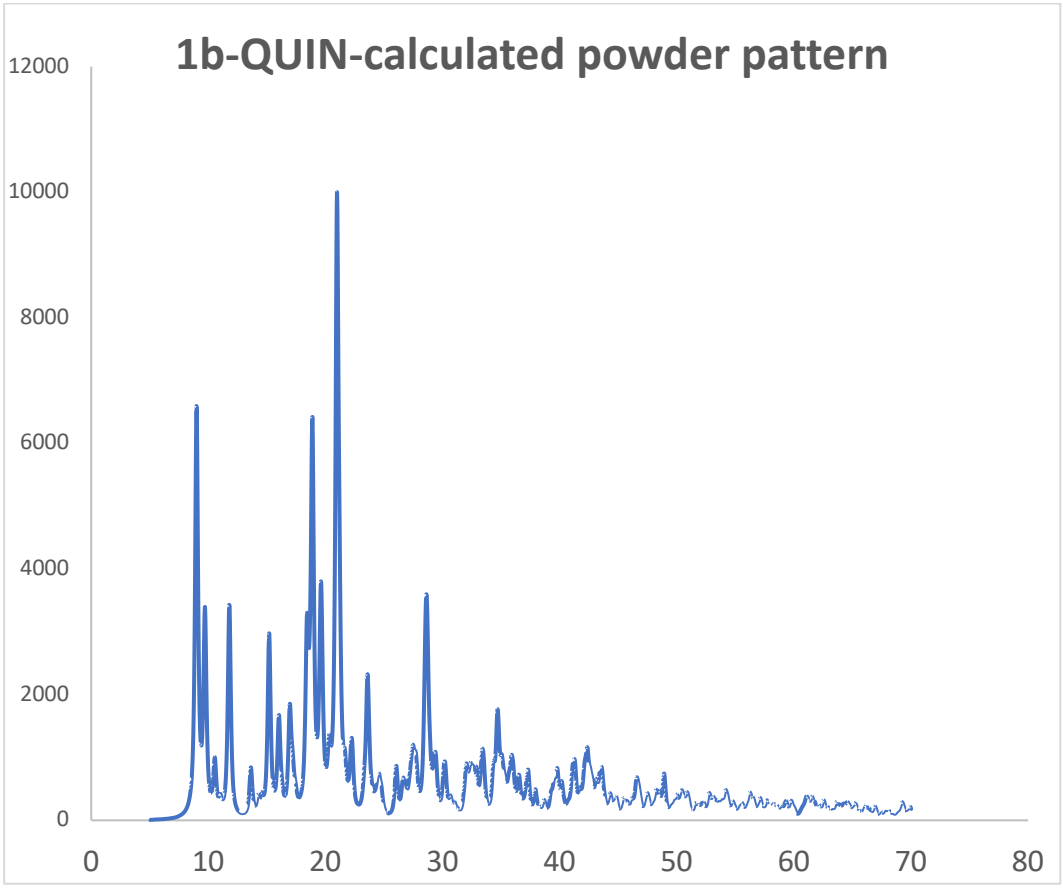

1b-DMAP-H2O-observed powder pattern
90
80
70
60
50
40
30
20
10
0
-10
0
10
20
30
40
50
60
70
80

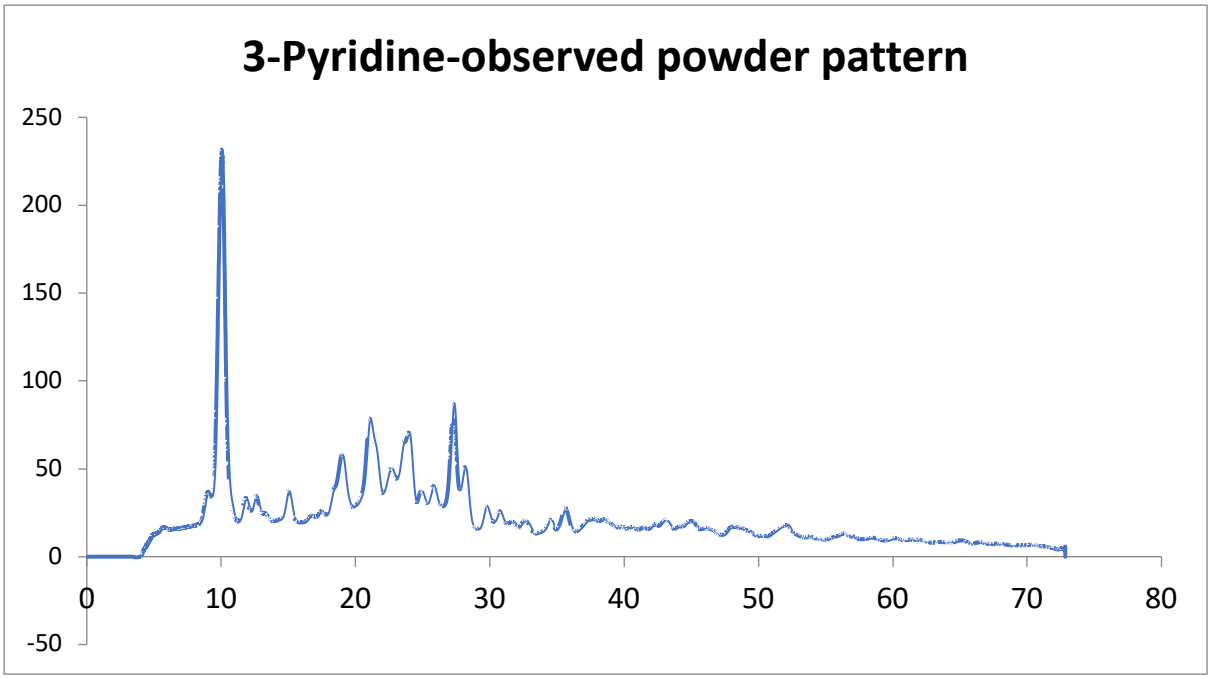

1b-DMAP-H2O-calculated powder pattern
12000
10000
8000
6000
4000
2000
0
0
10
20
30
40
50
60
70
80

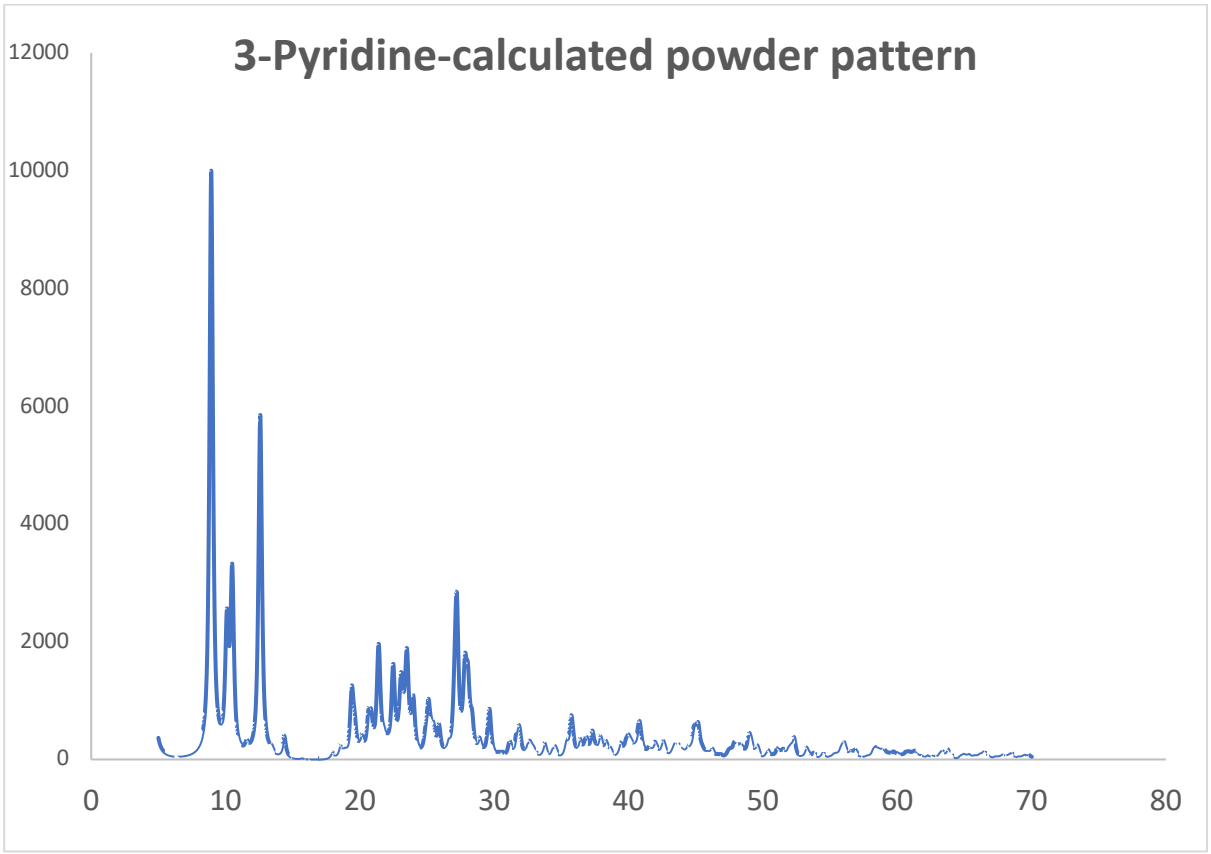

1b-DABCO-observed powder pattern
90
80
70
60
50
40
30
20
10
0
-10
0
10
20
30
40
50
60
70
80

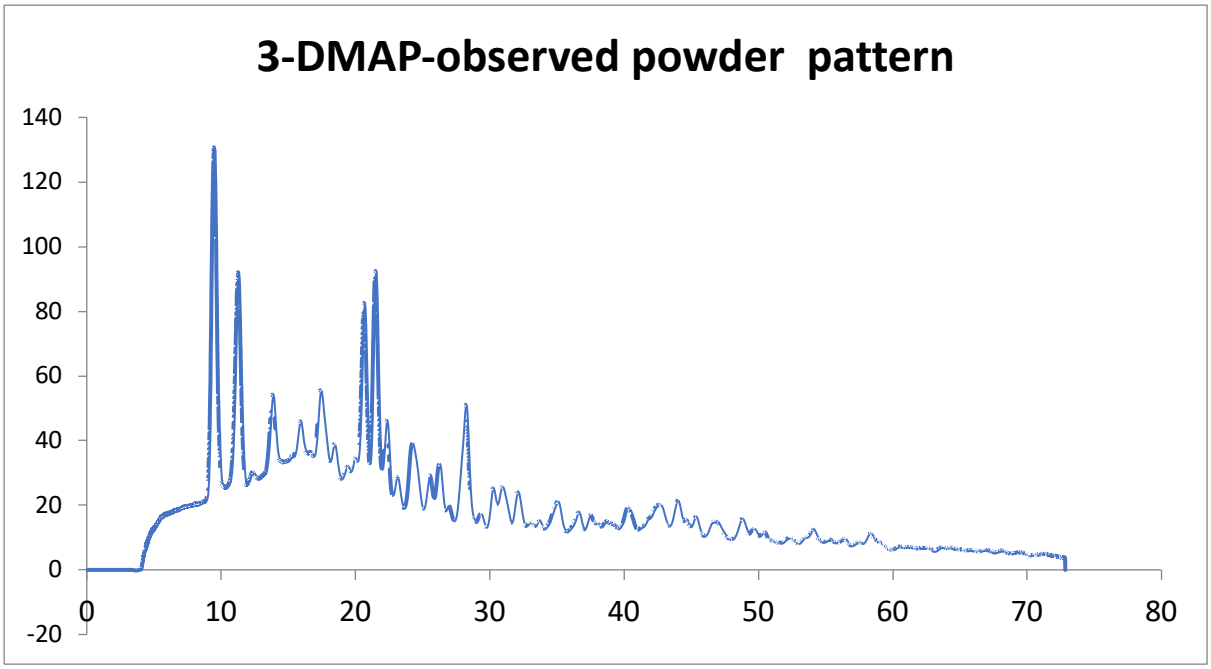

1b.DABCO-calculated powder pattern
12000
10000
8000
6000
4000
2000
0
0
10
20
30
40
50
60
70
80

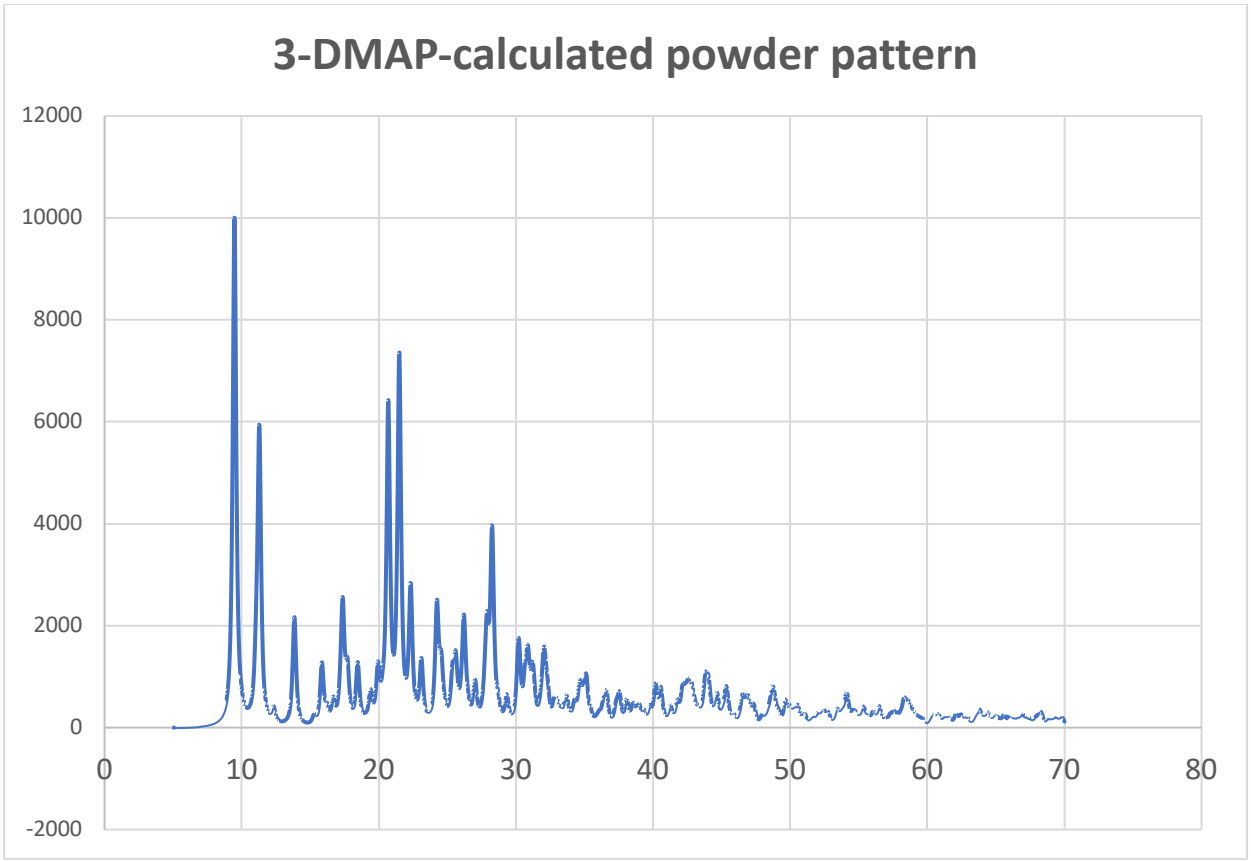

1b-QUIN-observed powder pattern
160
140
120
100
80
60
40
20
0
-20
0
20
40
60
80


1b-QUIN-calculated powder pattern
12000
10000
8000
6000
4000
2000
0
0
10
20
30
40
50
60
70
80


3-Pyridine-observed powder pattern
250
200
150
100
50
0
-50
0
10
20
30
40
50
60
70
80


3-Pyridine-calculated powder pattern
12000
10000
8000
6000
4000
2000
0
0
10
20
30
40
50
60
70
80


3-DMAP-observed powder pattern
140
120
100
80
60
40
20
0
-20
0
10
20
30
40
50
60
70
80


3-DMAP-calculated powder pattern
12000
10000
8000
6000
4000
2000
0
-2000
0
10
20
30
40
50
60
70
80

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