Electronic Supplementary Material (ESI) for CrystEngComm.
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Electronic Supplementary Information

On the inverse correlation between the hydrogen bond strength and chalcogen bond strength in the cyclic supramolecular heterosynthon [−Se−N=]···[HOOC−]

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1. Methods

1.1. Cocrystal synthesis

The 2,1,3-benzoselenadiazole (purity ⩾98%), *m*-nitrobenzoic acid (purity ⩾98%), *p*-nitrobenzoic acid (purity ⩾98%), 1,3,5-benzenetricarboxylic acid (purity ⩾98%), and the solvent methanol (analytical reagent grade) were purchased from Zhengzhou Alfa Chemical Co., Ltd., China. All of them were used as received. The 1:1 mixtures of 2,1,3-benzoselenadiazole (0.0183 g, 0.1 mmol) with *m*-nitrobenzoic acid (0.0167 g, 0.1 mmol), *p*-nitrobenzoic acid (0.0167 g, 0.1 mmol) and 1,3,5-benzenetricarboxylic acid (0.0210 g, 0.1 mmol), respectively, were dissolved in 15 mL of methanol, respectively. Upon slow evaporation of the solution at room temperature, cocrystals **I**, **II** and **III** suitable for single-crystal X-ray diffraction were obtained after 2–3 days.

1.2. Single-crystal X-ray diffraction

Single-crystal X-ray diffraction data were gathered on an Oxford Diffraction SuperNova area-detector diffractometer equipped with Mo-Kα X-ray source (λ = 0.71073 Å). The data reduction was treated by using CrysAlis Pro software.[1] The crystal structure was solved by SHELXS-2014 program.[2] Crystallographic data of cocrystals **I**, **II** and **III** were listed in Table S1. The CIF files of cocrystals **I**, **II** and **III** (CCDC deposition numbers: 2239190, 2239191 and 2239194) can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html. At the same time, the CIF files of cocrystals **I**, **II** and **III** were also provided as the electronic supplementary materials.

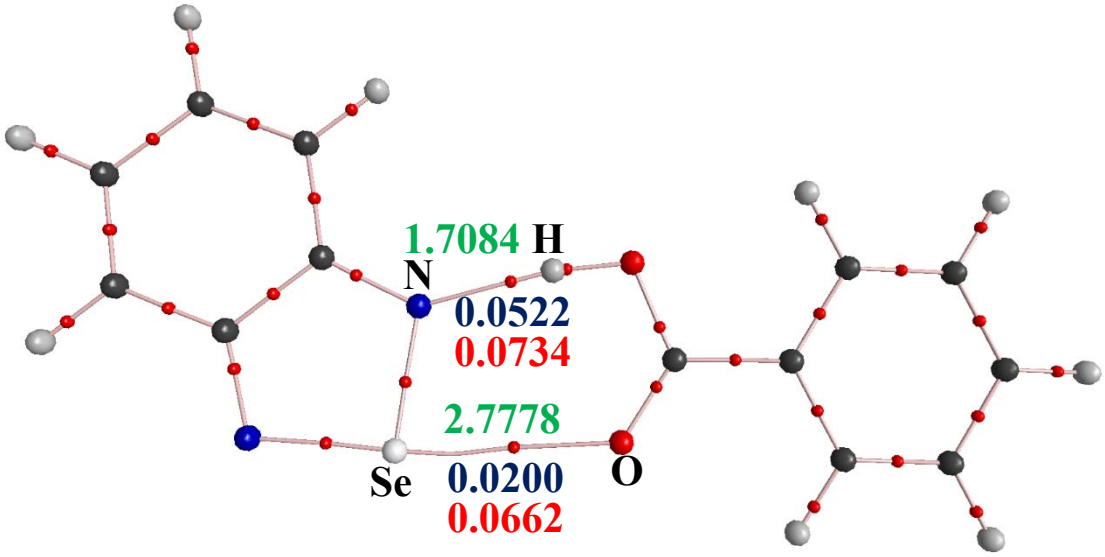
1.3. Computational details

The geometries of all the complexes were fully optimized at the PBE0-D3(BJ)/def2-TZVPP level of theory with the Gaussian 09 program.[3-7] All these optimized structures were confirmed to be energy minima by frequency calculations at the same theory level. Previous studies on the noncovalent interactions have shown that the PBE0-D3(BJ)/def2-TZVPP calculations can give comparable results with the “golden standard” coupled cluster calculations.[8,9]

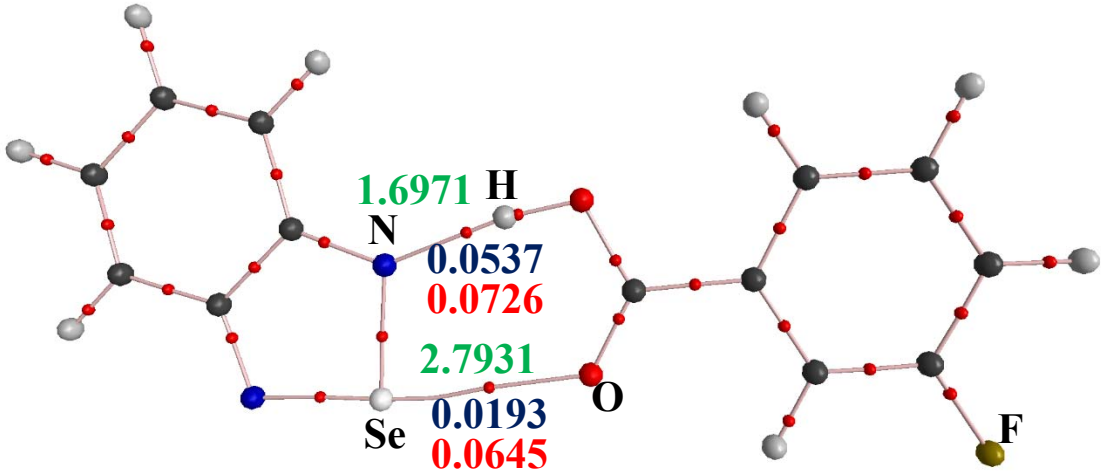
To further confirm the existence of the hydrogen bond and chalcogen bond in the cyclic supramolecular heterosynthon [−Se−N=]···[HOOC−], the "atoms in molecules" (AIM) analysis has been performed with the PBE0-D3(BJ)/def2-TZVPP electron density.[10] The AIM2000 software was employed to carry out the AIM analysis.[11] The analysis went further with those obtained by means of the natural bond orbital (NBO) theory of Weihnhold and co-workers.[12] The NBO analyses used the built-in subroutines of the Gaussian 09 program.

2. Table S1 Crystallographic data and structure refinement parameters for cocrystals I, II and III.

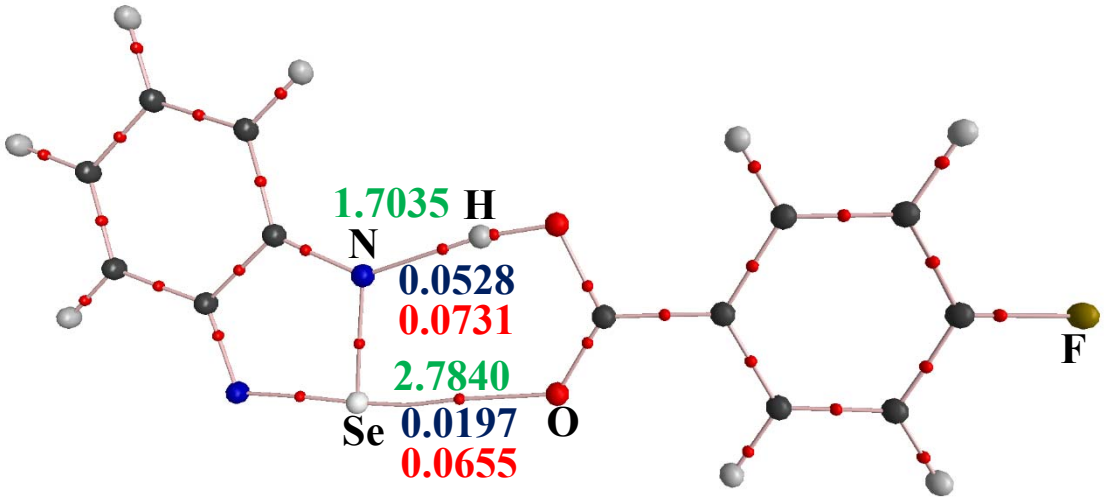
Cocrystal	I	II	III
CCDC No.	2239190	2239191	2239194
Empirical formula	$C_{13}H_9N_3O_4Se$	$C_{13}H_9N_3O_4Se$	$C_{27}H_{18}N_6O_6Se_3$
Formula weight	350.19	350.19	759.35
Crystal size/mm^3	0.28 × 0.25 × 0.24	0.25 × 0.24 × 0.23	0.24 × 0.21 × 0.2
Crystal system	triclinic	triclinic	monoclinic
Space group	*P*-1	*P*-1	$P2_1$
a/Å	6.6846(2)	6.7936(2)	3.9284(2)
b/Å	7.0498(2)	7.3480(3)	26.3154(12)
c/Å	15.0256(4)	14.7847(5)	13.1324(6)
α/°	97.105(2)	76.886(3)	90
β/°	94.771(2)	76.865(3)	91.977(4)
γ/°	109.331(3)	69.400(4)	90
V/Å^3	657.18(3)	663.98(4)	1356.79(11)
Z	2	2	2
ρ_{calc}/g·cm^{-3}	1.770	1.752	1.859
T/K	290	290	291
2*ϑ* range for data collection/°	6.516–56.938	6.66–56.7	6.928–57.062
Reflections collected	15586	15689	32014
Independent reflections [R_{int}]	3008 [0.0268]	3024 [0.0414]	6146 [0.0894]
R_1, wR_2 (I > 2σ(I))	0.0308, 0.0663	0.0414, 0.0932	0.0660, 0.1020
R_1, wR_2 (all data)	0.0371, 0.0684	0.0537, 0.0980	0.0936, 0.1107
Goodness-of-fit on F^2	1.097	1.092	1.059



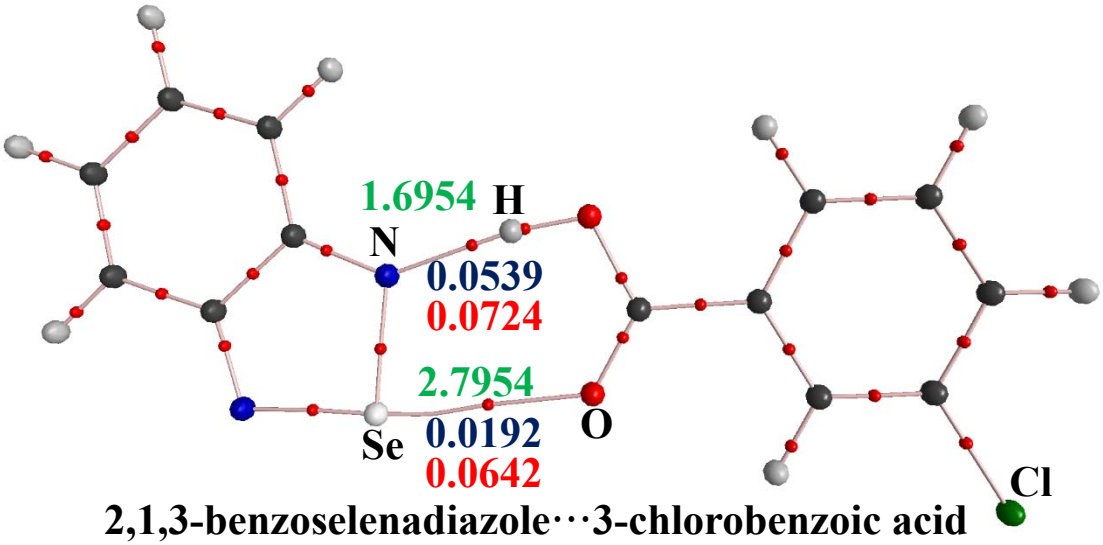
2,1,3-benzoselenadiazole···benzoic acid



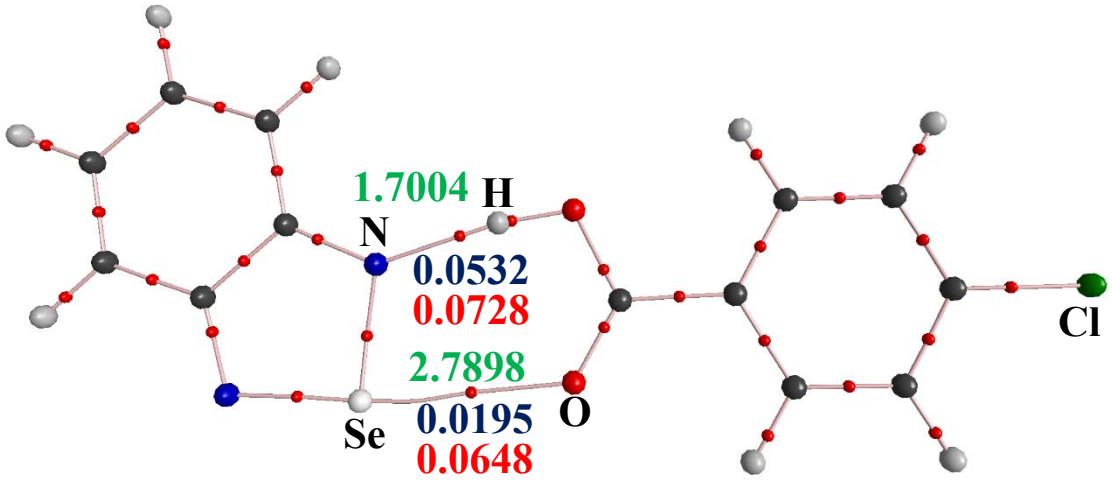
2,1,3-benzoselenadiazole···3-fluorobenzoic acid



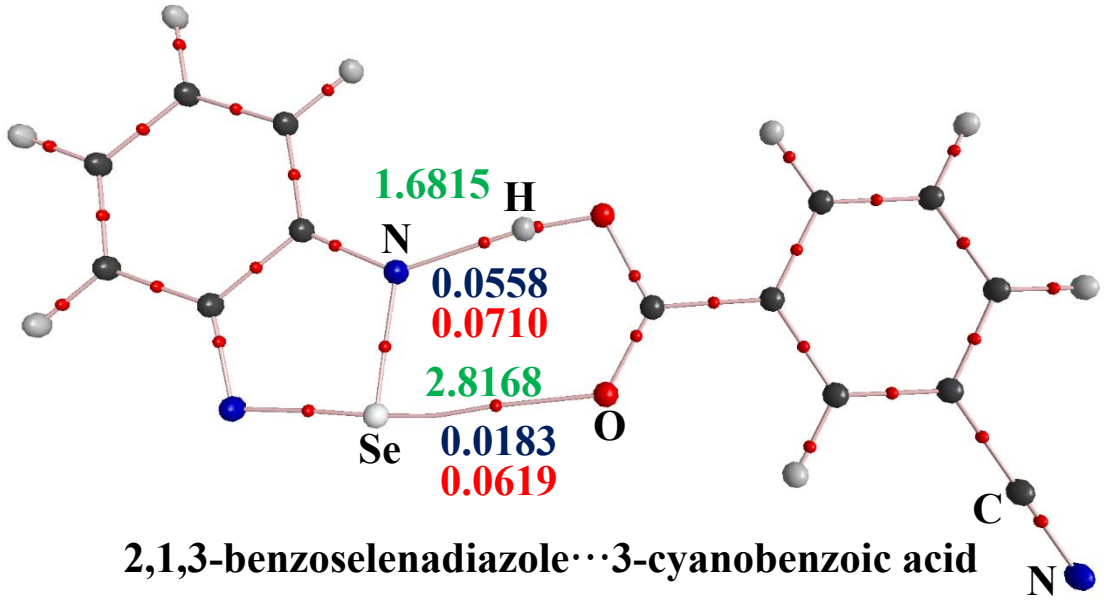
2,1,3-benzoselenadiazole···4-fluorobenzoic acid



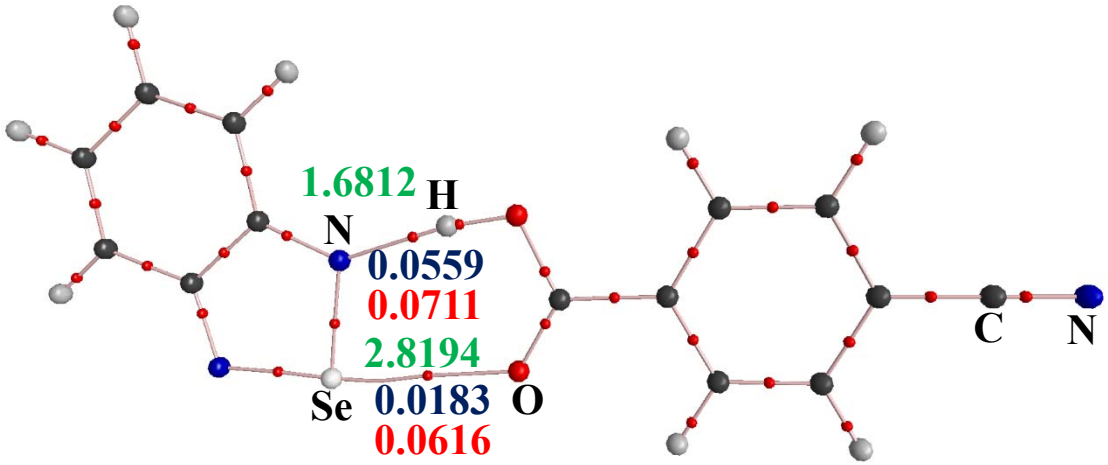
2,1,3-benzoselenadiazole···3-chlorobenzoic acid



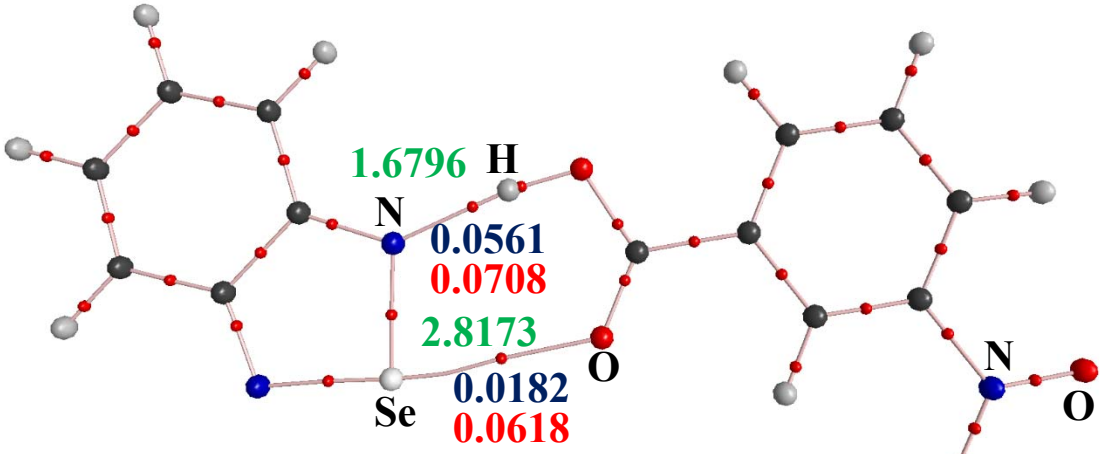
2,1,3-benzoselenadiazole···4-chlorobenzoic acid



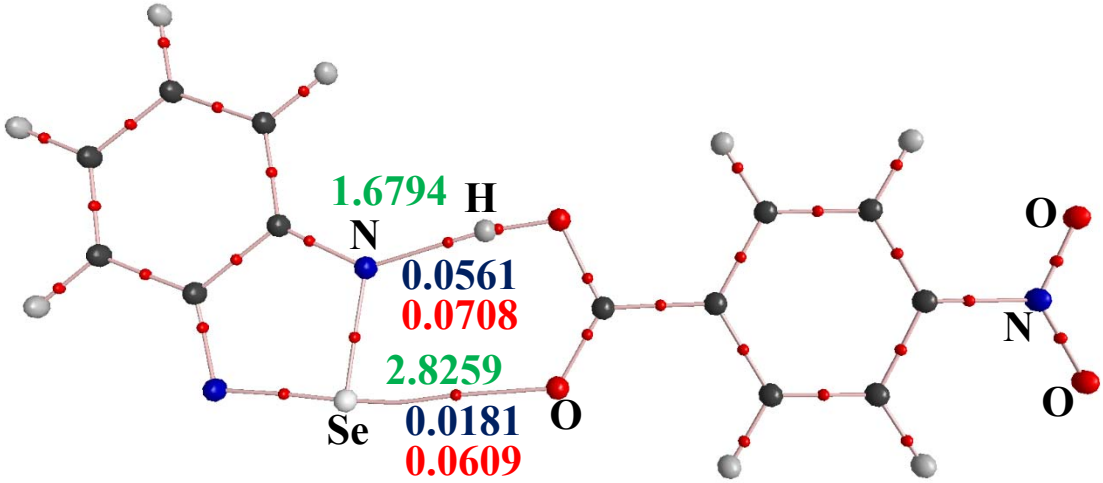
2,1,3-benzoselenadiazole···3-cyanobenzoic acid



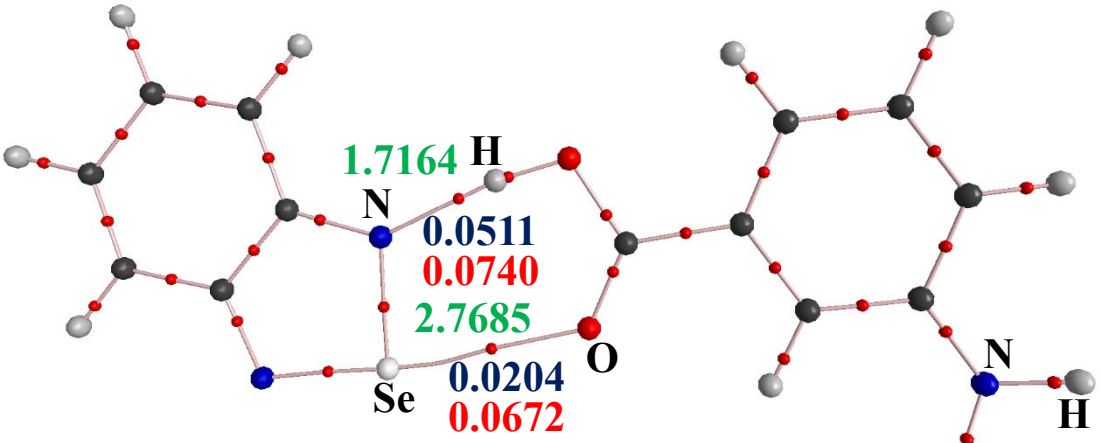
2,1,3-benzoselenadiazole···4-cyanobenzoic acid



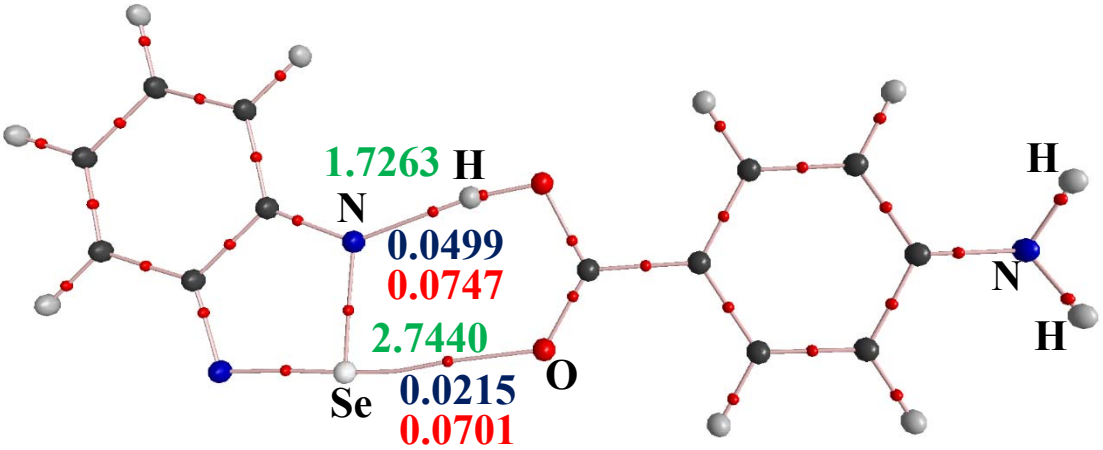
2,1,3-benzoselenadiazole···3-nitrobenzoic acid



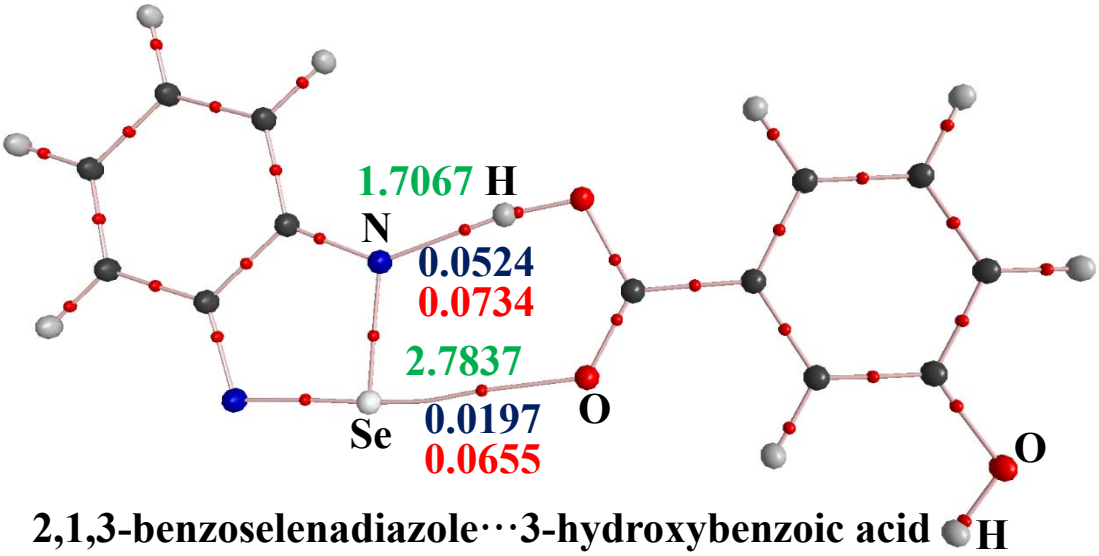
2,1,3-benzoselenadiazole···4-nitrobenzoic acid



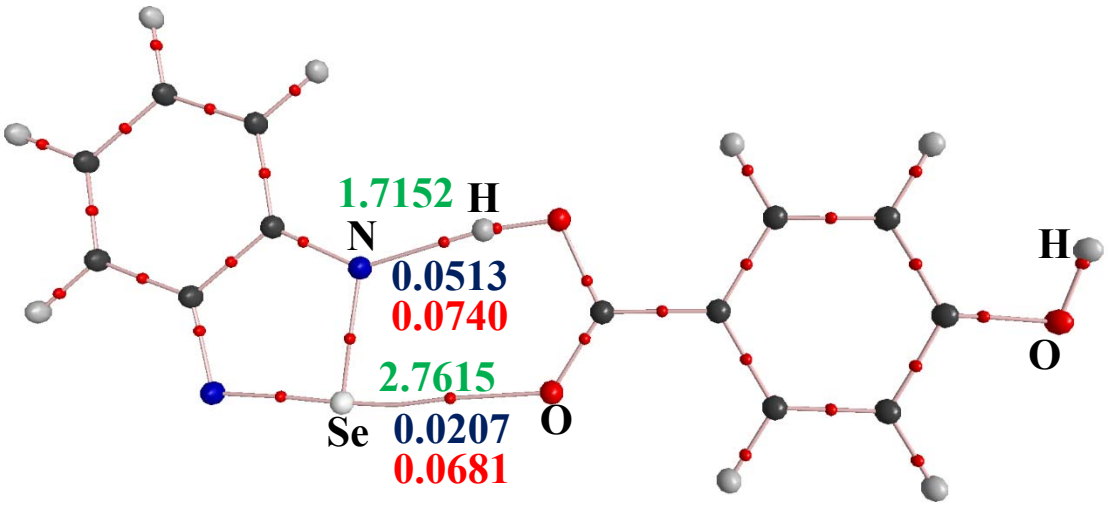
2,1,3-benzoselenadiazole···3-aminobenzoic acid



2,1,3-benzoselenadiazole···4-aminobenzoic acid



2,1,3-benzoselenadiazole···3-hydroxybenzoic acid



2,1,3-benzoselenadiazole···4-hydroxybenzoic acid

3. Fig. S1 The H···N and Se···O interatomic distances (green numbers, in Å) and the electron densities (blue numbers, in au) and their Laplacians (red numbers, in au) at the H···N and Se···O bond critical points in the cyclic supramolecular heterosynthons [–Se–N=]···[HOOC–] for the complexes formed between 2,1,3-benzoselenadiazole and a series of substituted and unsubstituted benzoic acid.

4. Cartesian coordinates for the π-stacked cluster formed by six 2,1,3-benzoselenadiazole molecules and six isophthalic acid molecules.

Se	-3.560425	-3.431732	0.279888
N	-4.737601	-3.538894	1.606806
C	-4.092291	-3.620722	2.757909
C	-4.701846	-3.702804	4.036953
H	-5.781038	-3.687977	4.114868
C	-3.898685	-3.794271	5.131299
H	-4.343084	-3.860371	6.116967
N	-2.194212	-3.521035	1.411320
C	-2.654758	-3.617485	2.646989
C	-1.854989	-3.715190	3.814911
H	-0.776670	-3.710422	3.724370
C	-2.478510	-3.805762	5.020178
H	-1.887319	-3.882423	5.924594
Se	8.360839	-3.055993	-2.055611
N	7.568862	-3.309544	-0.480377
C	8.511164	-3.600549	0.400481
C	8.286281	-3.841682	1.781518
H	7.279258	-3.792979	2.174400
C	9.357103	-4.108632	2.575222
H	9.206391	-4.281545	3.633804
N	9.975173	-3.380669	-1.418711
C	9.858351	-3.644137	-0.127862
C	10.943024	-3.939239	0.741755
H	11.948073	-3.966001	0.342280
C	10.684093	-4.159233	2.057385
H	11.501018	-4.366580	2.737245
Se	-2.605976	3.472567	0.844112
N	-3.746762	3.290767	2.194214
C	-3.070723	3.148762	3.321787
C	-3.645500	2.985367	4.608693
H	-4.722392	2.965005	4.713146
C	-2.813633	2.854076	5.676730
H	-3.231364	2.730316	6.668479
N	-1.209936	3.343307	1.934242
C	-1.636640	3.173388	3.173907
C	-0.805165	3.018370	4.313481
H	0.270137	3.019944	4.192241
C	-1.396854	2.865893	5.528975
H	-0.781453	2.748033	6.412575
Se	9.218434	2.768425	-1.693240
N	8.459565	2.989409	-0.097776

C	9.416282	2.940250	0.813335
C	9.210769	3.049001	2.213902
H	8.207961	3.184176	2.597095
C	10.290171	2.960451	3.035366
H	10.151640	3.028505	4.107462
N	10.844912	2.628113	-1.020605
C	10.752847	2.741338	0.294119
C	11.849509	2.664061	1.194820
H	12.845642	2.508753	0.802361
C	11.608262	2.768677	2.528064
H	12.430313	2.694095	3.228949
Se	-9.015546	-0.063944	1.007397
N	-10.502290	0.152934	0.080869
C	-10.173814	0.261539	-1.196685
C	-11.100686	0.450857	-2.256626
H	-12.155782	0.515118	-2.028169
C	-10.622554	0.546715	-3.525442
H	-11.312972	0.690832	-4.347544
N	-7.975679	0.003330	-0.434338
C	-8.757278	0.178009	-1.487206
C	-8.305042	0.282706	-2.827937
H	-7.245906	0.217325	-3.039239
C	-9.228996	0.461601	-3.809076
H	-8.903074	0.543175	-4.839140
Se	3.065939	0.219120	-0.120534
N	1.740296	0.405681	-1.284349
C	2.237549	0.471079	-2.508032
C	1.477784	0.624819	-3.695791
H	0.400377	0.700927	-3.632006
C	2.139042	0.673500	-4.882698
H	1.578868	0.791489	-5.802337
N	4.283441	0.238977	-1.414944
C	3.675495	0.374983	-2.581934
C	4.325144	0.427401	-3.841959
H	5.403074	0.353181	-3.888385
C	3.557816	0.573034	-4.955580
H	4.032460	0.616834	-5.928317
O	-6.046469	-3.418456	-1.106918
O	-7.275993	-3.460529	0.757027
H	-6.361640	-3.489861	1.164892
C	-9.622437	-3.214016	-0.627913
H	-9.648434	-3.243677	0.451250
C	-8.408388	-3.315844	-1.294275
C	-8.372074	-3.284160	-2.683698

H	-7.410372	-3.360852	-3.174821
C	-9.544012	-3.141210	-3.407662
H	-9.513344	-3.113094	-4.489412
C	-7.127625	-3.408012	-0.550383
O	-13.116047	-2.540722	-1.268641
O	-12.047328	-2.989148	0.639381
H	-12.931637	-2.790161	0.968455
C	-10.792688	-3.041817	-1.354611
C	-10.751422	-3.005761	-2.745562
H	-11.677770	-2.858702	-3.285417
C	-12.099259	-2.831879	-0.692605
O	5.674717	-2.769103	-2.771800
O	4.898901	-3.159768	-0.715431
H	5.881305	-3.188258	-0.522506
C	2.283567	-3.055972	-1.550997
H	2.485521	-3.147430	-0.493682
C	3.332016	-2.949181	-2.455036
C	3.068658	-2.838829	-3.817578
H	3.905034	-2.754260	-4.498710
C	1.762521	-2.834926	-4.274524
H	1.559708	-2.746928	-5.334276
C	4.745540	-2.947845	-2.004908
O	-1.329881	-3.192214	-1.458858
O	0.175417	-3.230339	0.189757
H	-0.661544	-3.338111	0.727280
C	0.972895	-3.043086	-2.011575
C	0.715143	-2.934333	-3.373566
H	-0.316138	-2.930633	-3.703066
C	-0.175463	-3.158681	-1.078187
O	-5.123390	3.606173	-0.469196
O	-6.304306	3.267714	1.395559
H	-5.379866	3.254014	1.780445
C	-8.696030	3.448072	0.071407
H	-8.696782	3.292795	1.140292
C	-7.491046	3.568437	-0.609241
C	-7.485800	3.773348	-1.984223
H	-6.531062	3.863231	-2.486664
C	-8.680192	3.855552	-2.680928
H	-8.673835	4.011378	-3.752161
C	-6.190149	3.483071	0.100771
O	-12.260223	3.315200	-0.543741
O	-11.109664	3.235751	1.367657
H	-12.007032	3.087580	1.688139
C	-9.892032	3.518822	-0.630782

C	-9.881658	3.724298	-2.008055
H	-10.828742	3.768567	-2.529396
C	-11.204155	3.350646	0.033542
O	6.537265	3.191963	-2.429153
O	5.817570	3.359461	-0.321955
H	6.790268	3.197409	-0.143848
C	3.208689	3.644942	-1.113869
H	3.419329	3.485064	-0.066690
C	4.242377	3.645069	-2.039707
C	3.969364	3.854308	-3.388113
H	4.792831	3.838793	-4.090187
C	2.667668	4.067630	-3.807931
H	2.457165	4.234458	-4.856718
C	5.641377	3.379859	-1.625539
O	-0.397533	3.806031	-0.943517
O	1.136787	3.531599	0.656210
H	0.309130	3.446926	1.211766
C	1.899385	3.819984	-1.542412
C	1.631701	4.039112	-2.888921
H	0.601614	4.171488	-3.194639
C	0.764091	3.726360	-0.591683
O	0.691698	0.117517	1.620027
O	-0.677329	0.230724	-0.142687
H	0.192352	0.329808	-0.627709
C	-2.909956	-0.061920	1.375689
H	-3.003991	0.050596	0.305661
C	-1.653004	-0.065145	1.965153
C	-1.534060	-0.213938	3.343091
H	-0.542970	-0.214623	3.778224
C	-2.667026	-0.354266	4.127106
H	-2.572523	-0.468473	5.198998
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H	12.426684	-0.677517	-0.443386
C	9.057746	-0.373643	1.018817
H	9.138338	-0.321604	-0.057729

C	10.191719	-0.550943	1.799659
C	10.080532	-0.616878	3.184765
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C	7.706908	-0.334454	3.009150
H	6.722944	-0.250742	3.453096
C	6.572046	-0.095239	0.825484

Notes and references

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5. The CheckCIF reports for cocrystals I, II and III.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2239190, 2239191, 2239194

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2239190

Bond precision: C-C = 0.0034 A Wavelength=0.71073

Cell: a=6.6846(2) b=7.0498(2) c=15.0256(4)
alpha=97.105(2) beta=94.771(2) gamma=109.331(3)
Temperature: 290 K

	Calculated	Reported
Volume	657.18(4)	657.18(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C7 H5 N O4, C6 H4 N2 Se	C6 H4 N2 Se, C7 H5 N O4
Sum formula	C13 H9 N3 O4 Se	C13 H9 N3 O4 Se
Mr	350.19	350.19
Dx,g cm-3	1.770	1.770
Z	2	2
Mu (mm-1)	2.877	2.877
F000	348.0	348.0
F000'	347.97	
h,k,lmax	8,9,20	8,9,19
Nref	3319	3008
Tmin,Tmax	0.451,0.501	0.754,1.000
Tmin'	0.442	

Correction method= # Reported T Limits: Tmin=0.754 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.906 Theta(max)= 28.469

R(reflections)= 0.0308(2720) wR2(reflections)= 0.0684(3008)

S = 1.097 Npar= 191

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.561 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
```

Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        304 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          7 Info
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
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5 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: 2239191

Bond precision: C-C = 0.0045 A Wavelength=0.71073

Cell:	a=6.7936(2)	b=7.3480(3)	c=14.7847(5)
	alpha=76.886(3)	beta=76.865(3)	gamma=69.400(4)
Temperature:	290 K		

	Calculated	Reported
Volume	663.98(4)	663.98(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C7 H5 N O4, C6 H4 N2 Se	C6 H4 N2 Se, C7 H5 N O4
Sum formula	C13 H9 N3 O4 Se	C13 H9 N3 O4 Se
Mr	350.19	350.19
Dx,g cm-3	1.752	1.752
Z	2	2
Mu (mm-1)	2.848	2.848
F000	348.0	348.0
F000'	347.97	
h,k,lmax	9,9,19	8,9,19
Nref	3319	3024
Tmin,Tmax	0.496,0.519	0.729,1.000
Tmin'	0.486	

Correction method= # Reported T Limits: Tmin=0.729 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.911 Theta(max)= 28.350

R(reflections)= 0.0414(2581) wR2(reflections)= 0.0980(3024)

S = 1.092 Npar= 191

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density .... 4.05 Report
PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree

---

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.000 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note

---

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 1 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 281 Note

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 7 Info

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5 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: 2239194

Bond precision: C-C = 0.0160 A Wavelength=0.71073

Cell: a=3.9284(2) b=26.3154(12) c=13.1324(6)
alpha=90 beta=91.977(4) gamma=90
Temperature: 291 K

	Calculated	Reported
Volume	1356.79(11)	1356.79(11)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C9 H6 O6, 3(C6 H4 N2 Se)	3(C6 H4 N2 Se), C9 H6 O6
Sum formula	C27 H18 N6 O6 Se3	C27 H18 N6 O6 Se3
Mr	759.35	759.35
Dx,g cm-3	1.859	1.859
Z	2	2
Mu (mm-1)	4.122	4.122
F000	744.0	744.0
F000'	743.76	
h,k,lmax	5,35,17	5,34,17
Nref	6915[3532]	6146
Tmin,Tmax	0.387,0.438	0.554,1.000
Tmin'	0.358	

Correction method= # Reported T Limits: Tmin=0.554 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.74/0.89 Theta(max)= 28.531

R(reflections)= 0.0660(4825) wR2(reflections)= 0.1107(6146)

S = 1.059 Npar= 381

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT430_ALERT_2_A Short Inter D...A Contact Se2 ..N1 . 2.90 Ang.
-x,1/2+y,2-z = 2_557 Check

Author Response: The Checkcif software has a bug and cannot identify chalcogen bonds.

PLAT430_ALERT_2_A Short Inter D...A Contact Se3 ..O3 . 2.82 Ang.
x,y,z = 1_555 Check

Author Response: The Checkcif software has a bug and cannot identify chalcogen bonds.

Alert level B

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.01596 Ang.
PLAT927_ALERT_1_B Reported and Calculated wR2 Differ by ..... 0.0095 Check

---

Alert level C

STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.452
From the CIF: _refine_ls_abs_structure_Flack_su 0.008
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT234_ALERT_4_C Large Hirshfeld Difference C25 --C26 . 0.17 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.978 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 8 Note
PLAT926_ALERT_1_C Reported and Calculated R1 Differ by ..... 0.0048 Check
PLAT987_ALERT_1_C The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

---

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 3 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.452 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C6 H4 N2 Se
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3 Note
C6 H4 N2 Se
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 252 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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```
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```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

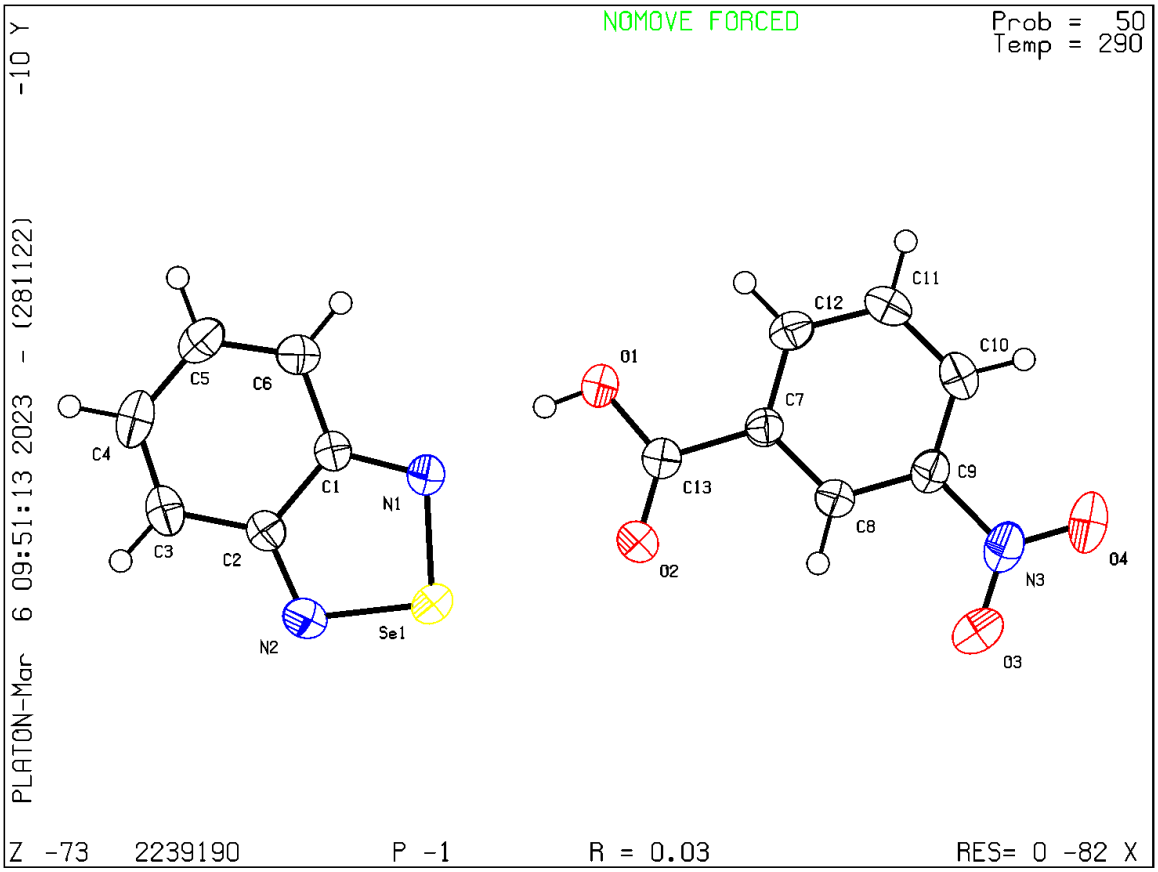
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

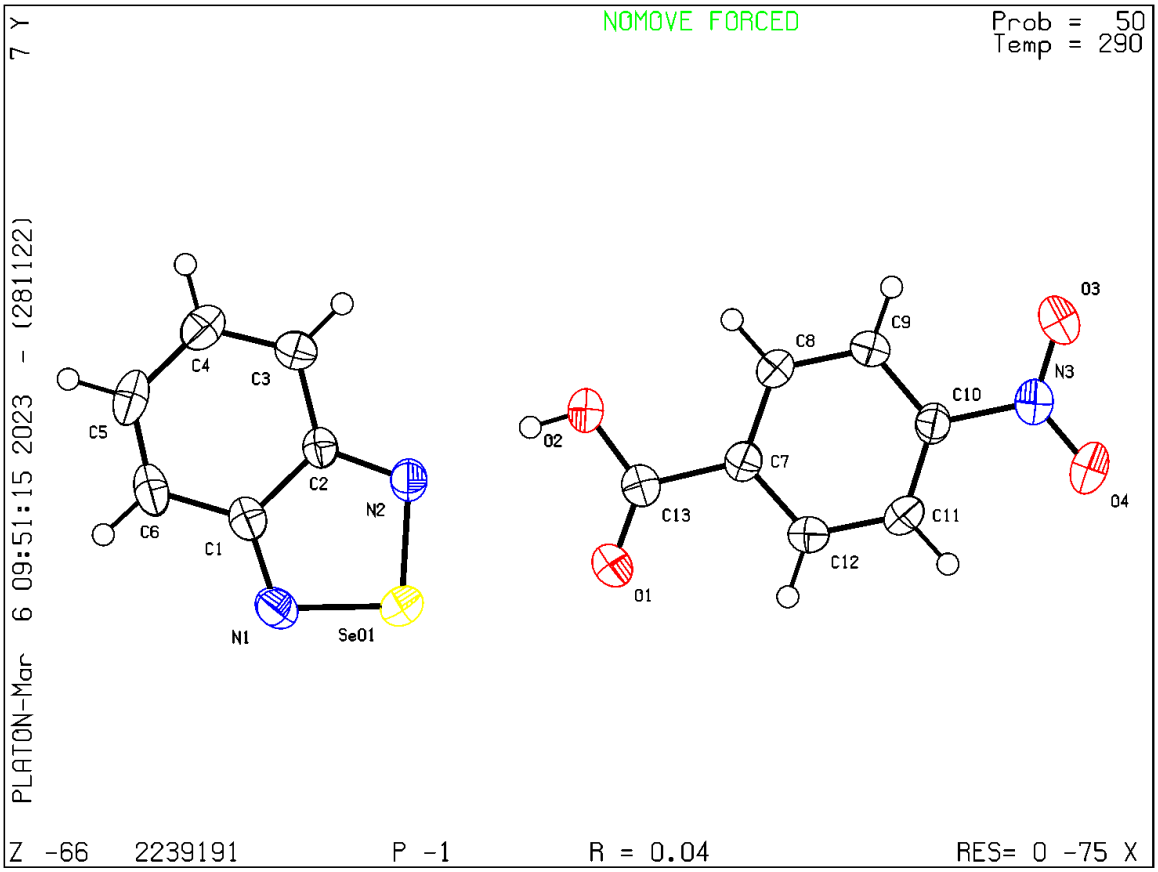
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock 2239190 - ellipsoid plot



Datablock 2239191 - ellipsoid plot



Datablock 2239194 - ellipsoid plot