

Supplementary Information

Intrinsic Influence of Selenium Substitution on Electronic Structure, Excited States and Photovoltaic Performances Evaluated by Theoretical Calculation

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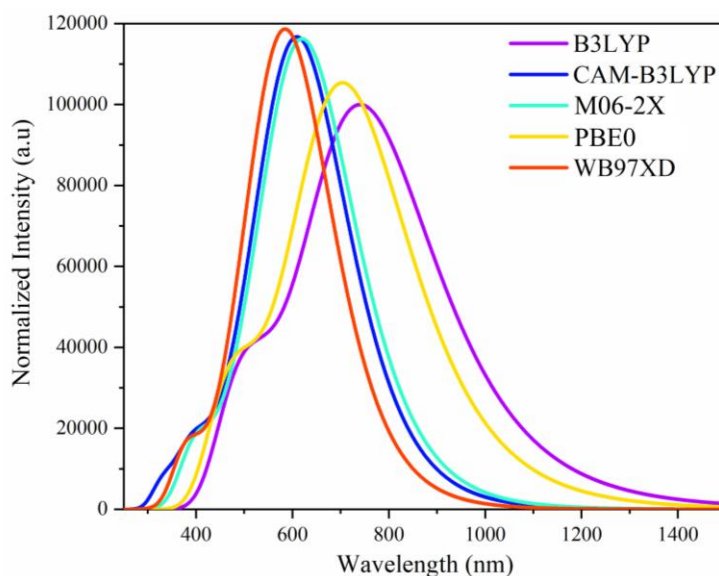


Fig. S1 Theoretical observed absorption spectra of Y6 with B3LYP, CAM-B3LYP, ω B97XD, PBE0 and M06-2X functionals.

Table S1

Experimental and calculated λ_{max} values of Y6 with B3LYP, CAM-B3LYP, ω B97XD, PBE0 and M062X functionals in def2-TZVP level.

Hybird functionals	Calc. λ_{max} (nm) /Exp. λ_{max} (nm)	Err. λ_{max} (nm)
B3LYP	750.51/731	19.51
CAM-B3LYP	620.91	110.09
ω B97XD	597.37	133.63
PBE0	713.13	17.87
M06-2X	631.70	93.30

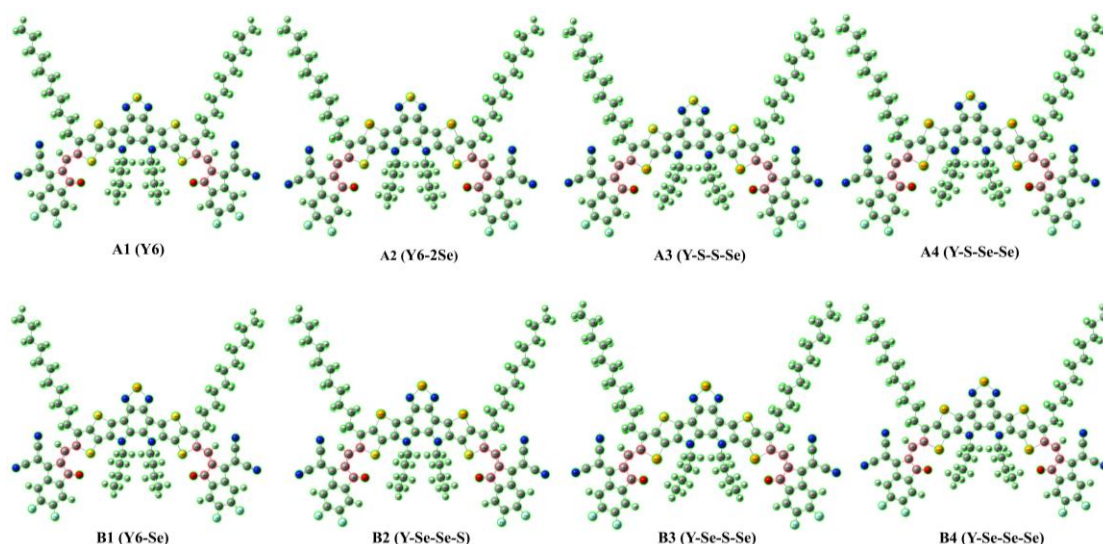


Fig. S2 Optimized geometric structures atomic number marking of Y6 and its derivatives (red marks atoms associated with dihedral angles and green marks other atoms).

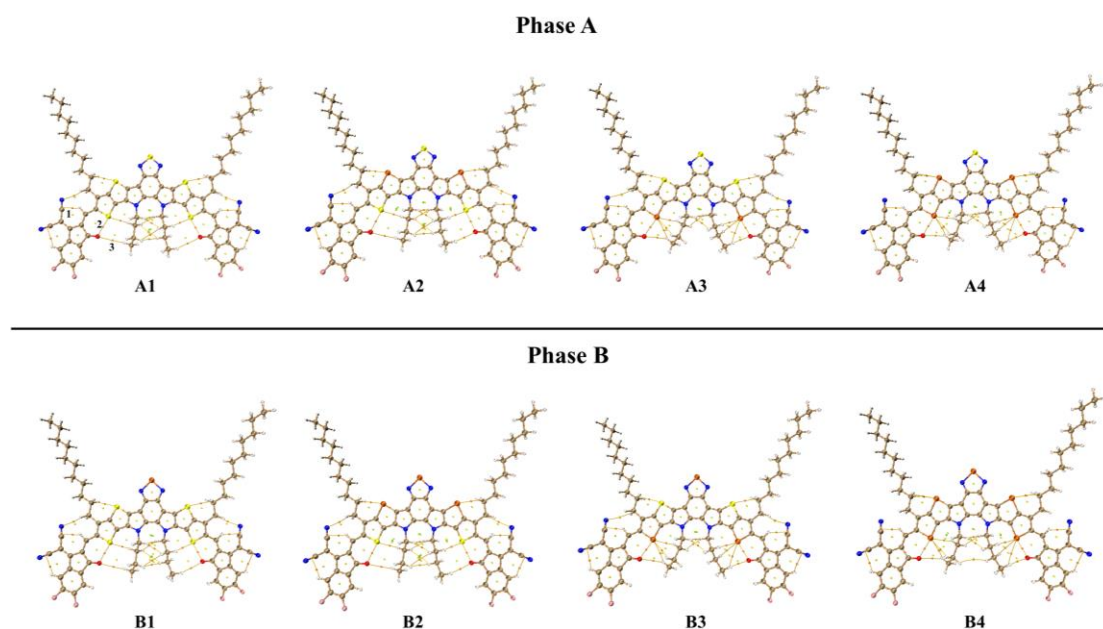


Fig. S3 Topological analysis of the intramolecular bond critical point (3, -1) based on AIM theory for molecules Phase A and B.

Table S2

Lagrangian kinetic energy $G(r)$, Energy density $E(r)$, Potential energy density $V(r)$, Electron Density ρ and Laplacian of Electron Density $\nabla^2\rho$ at the Intramolecular Bond Critical Point (3, -1) with the $H\cdots\pi$, $S\cdots O$, $Se\cdots O$, and Associated $H\cdots H$ Interactions of molecules.

	A1			A2			A3			A4		
	$H\cdots\pi$	$S\cdots O$	$H\cdots H$	$H\cdots\pi$	$S\cdots O$	$H\cdots H$	$H\cdots\pi$	$Se\cdots O$	$H\cdots H$	$H\cdots\pi$	$Se\cdots O$	$H\cdots H$
$G(r)$	0.013	0.019	0.009	0.013	0.019	0.009	0.013	0.025	0.008	0.013	0.024	0.009
$E(r)$	0.002	0.001	0.002	0.002	0.001	0.002	0.002	0.000	0.002	0.002	0.000	0.002
$-V(r)$	0.011	0.018	0.007	0.011	0.018	0.007	0.011	0.025	0.007	0.011	0.024	0.007
ρ	0.018	0.023	0.012	0.019	0.024	0.012	0.019	0.031	0.011	0.019	0.031	0.011

$\nabla^2\rho$	0.059	0.080	0.042	0.062	0.081	0.042	0.061	0.098	0.039	0.061	0.098	0.041
	B1		B2			B3			B4			
	H $\cdots\pi$	S \cdots O	H \cdots H	H $\cdots\pi$	S \cdots O	H \cdots H	H $\cdots\pi$	Se \cdots O	H \cdots H	H $\cdots\pi$	Se \cdots O	H \cdots H
G(r)	0.013	0.019	0.009	0.013	0.019	0.009	0.013	0.025	0.008	0.013	0.024	0.002
E(r)	0.002	0.001	0.002	0.002	0.001	0.002	0.002	0.000	0.002	0.002	0.000	0.002
-V(r)	0.011	0.018	0.007	0.011	0.018	0.008	0.011	0.024	0.007	0.011	0.024	0.008
ρ	0.019	0.024	0.111	0.019	0.024	0.012	0.019	0.025	0.011	0.019	0.031	0.012
$\nabla^2\rho$	0.062	0.081	0.041	0.062	0.080	0.042	0.061	0.098	0.039	0.061	0.098	0.042

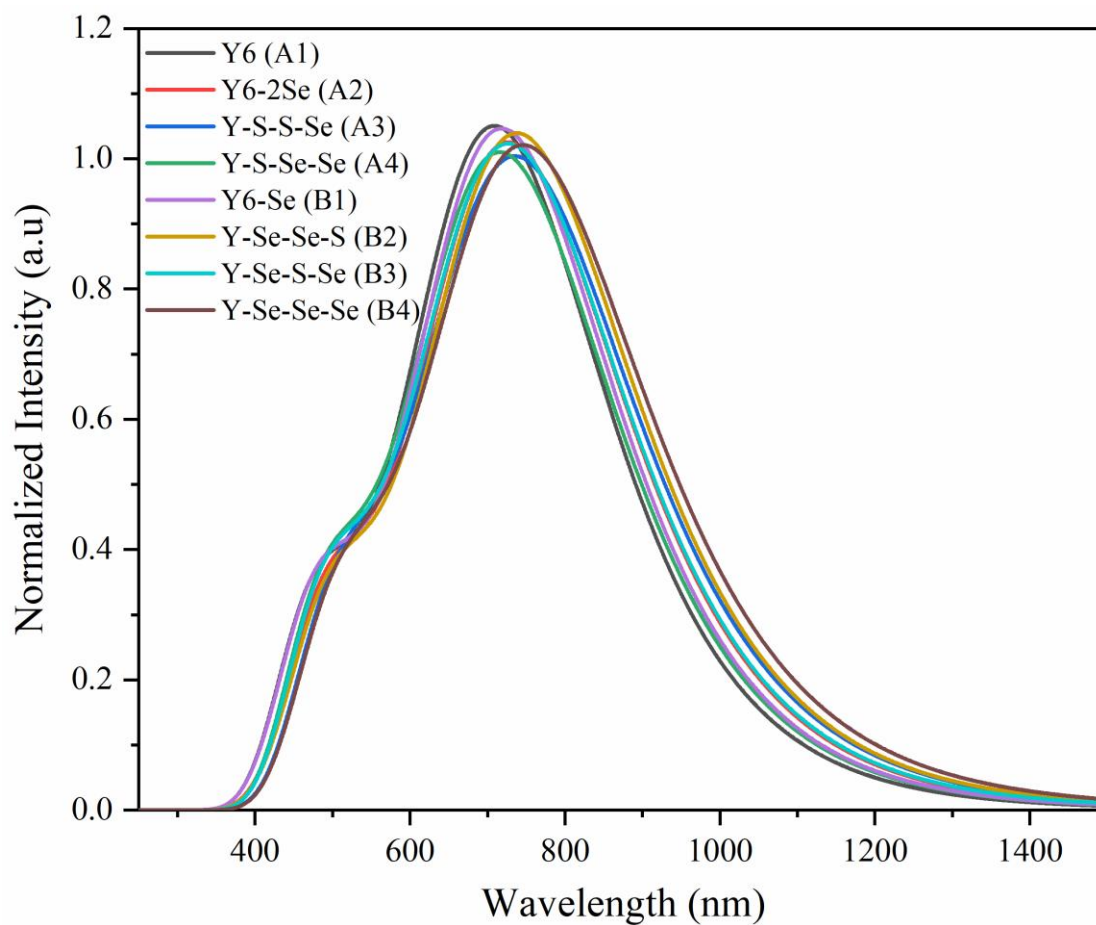


Fig. S4 Simulated absorption spectra in the solvent(chloroform) of Y6 series molecules calculated at the PBE0 with def2-TZVP basis set.

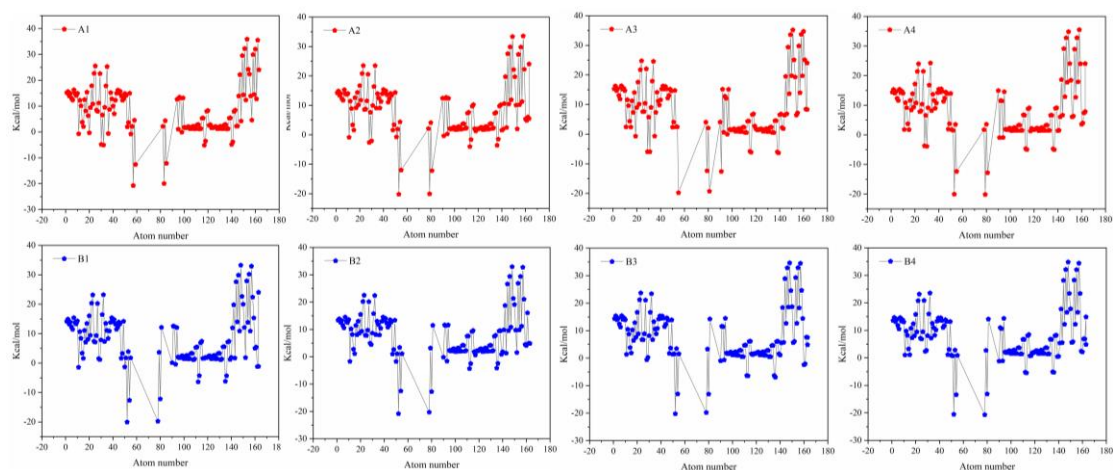


Fig. S5 The averaged ESP values of the atoms in all molecules.

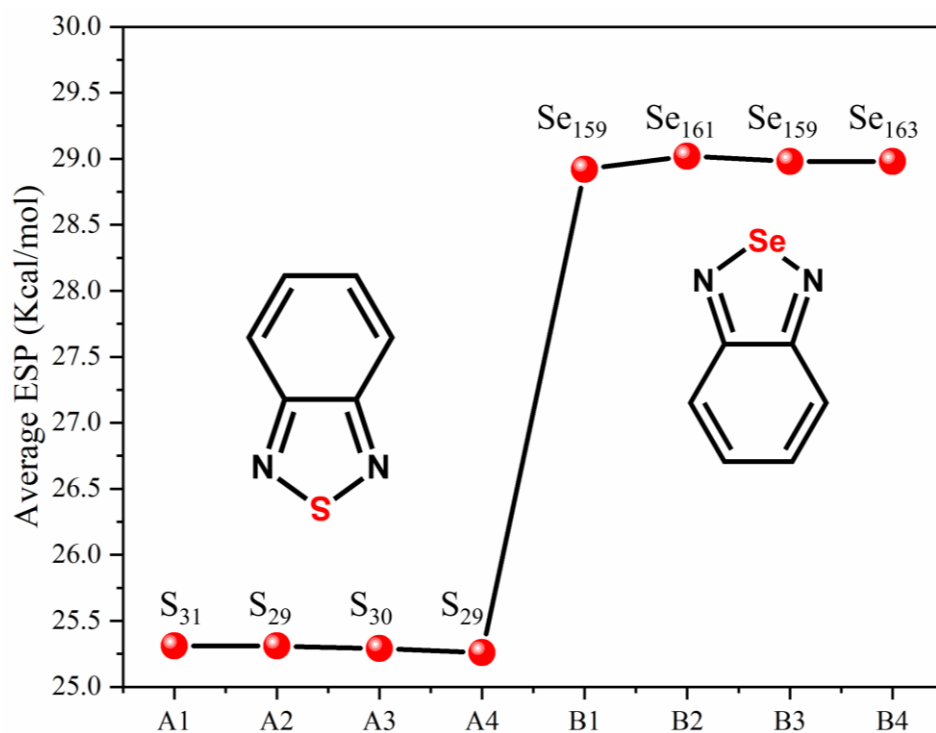


Fig. S6 The average electrostatic potential values of the S position in Benzothiadiazole in series A and the position of Benzoselenadiazole Se in series B.

Table S3

Molecular surface area, molecular polarity index (MPI), extreme value of ESP and total average ESPs of Y6 series molecules (isosurface = 0.001 a.u.).

Molecules	A1	A2	A3	A4	B1	B2	B3	B4
Overall surface area/ \AA^2	1313.68	1304.50	1297.89	1301.40	1309.47	1309.15	1301.99	1306.46
Molecular polarity index/kcal mol ⁻¹	10.70	10.49	10.68	10.71	10.38	10.44	10.62	10.66
Minimal value/kcal mol ⁻¹	-39.15	-39.15	-38.83	-39.33	-39.13	-39.64	-39.34	-39.80
Maximal value/kcal mol ⁻¹	43.94	41.46	44.82	43.87	41.68	40.82	44.10	43.22
Overall average value/kcal mol ⁻¹	5.42	5.57	5.53	5.74	5.19	5.41	5.38	5.60

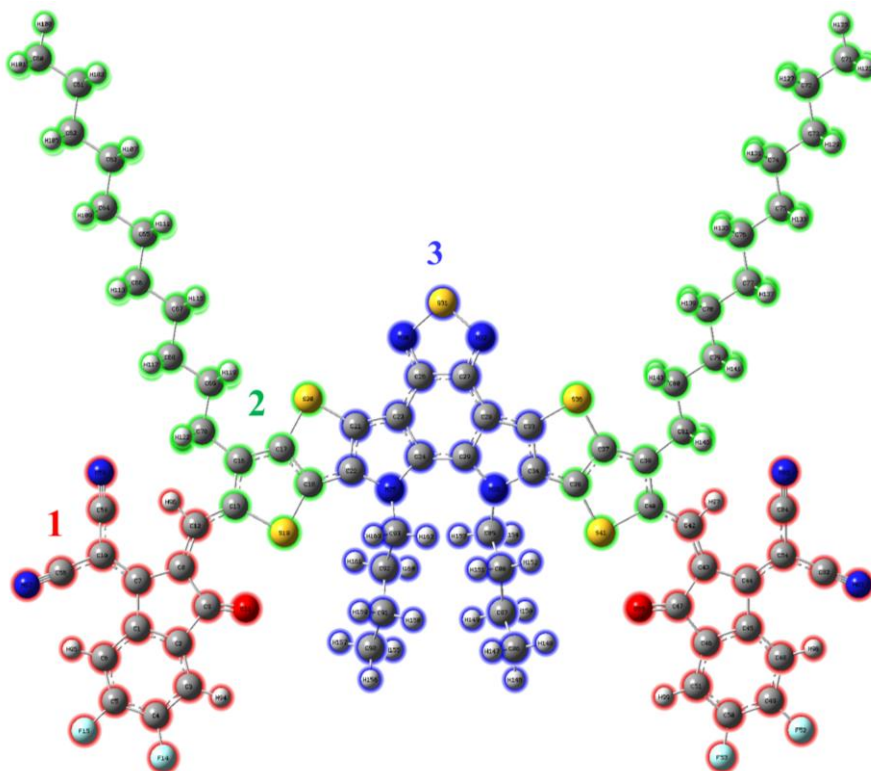


Fig. S7 Three segments of Y6 and fragments 1, 2 and 3 are two end groups (A), two donor units (D) and acceptor center core (A') respectively.

Table S4

Percentage of charge transfer for different fragments, Intrinsic local excitation percentage and Intrinsic charge transfer percentage of the molecules.

Molecules	2->1(%)	3->1(%)	3->2(%)	CT (%)	LE (%):
A1	27.602%	11.833%	6.573%	61.486%	33.417%
A2	28.075%	11.557%	6.409%	61.587%	33.536%
A3	27.431%	10.834%	6.480%	60.566%	33.659%
A4	27.823%	10.513%	6.348%	60.478%	33.976%
B1	27.104%	12.428%	6.900%	61.902%	33.039%
B2	27.430%	12.138%	6.733%	61.849%	33.249%
B3	26.712%	11.366%	6.816%	60.777%	33.423%
B4	27.108%	11.073%	6.690%	60.727%	33.738%

Below are the XYZ coordinates of the six molecules

Y6(A1)

C	9.49763200	-5.17772900	-0.63675600
C	8.14889800	-5.56437200	-0.63175700
C	7.74360700	-6.88320200	-0.74988300
C	8.73504200	-7.84067300	-0.87730500
C	10.08235900	-7.47380800	-0.88440100
C	10.48820000	-6.15300700	-0.76596000

C	9.56947500	-3.70019000	-0.49131900
C	8.20130100	-3.20614300	-0.39634300
C	7.29403100	-4.36436000	-0.48451400
C	10.75025100	-2.98161600	-0.45992800
O	6.07341300	-4.36694700	-0.44510000
C	7.82813400	-1.88147200	-0.24300000
C	6.60281000	-1.20764100	-0.13420900
F	8.41954700	-9.13772900	-0.99622300
F	11.00378400	-8.43949300	-1.01031600
C	6.54341700	0.20776800	0.02983700
C	5.18905632	0.72600588	0.11757742
C	4.26111800	-0.37754800	0.02004700
S	4.98305900	-1.93669500	-0.17424700
S	4.43764168	2.31815512	0.29223558
C	2.77489000	1.45340900	0.21866200
C	2.92697200	0.06954200	0.09658300
C	1.40387200	1.73627600	0.16236000
C	0.71695900	0.48883800	0.03392600
N	1.67454000	-0.52245800	-0.01217200
C	0.71191100	2.98296800	0.11250700
C	-0.71192300	2.98296900	-0.11251100
C	-1.40388300	1.73627900	-0.16240100
C	-0.71696300	0.48883700	-0.03400200
N	1.24377500	4.19262900	0.19396800
S	-0.00000800	5.27431000	0.00003000
N	-1.24378700	4.19263200	-0.19394200
C	-2.77489900	1.45341000	-0.21870700
C	-2.92697800	0.06954200	-0.09662200
N	-1.67454600	-0.52245000	0.01213600
S	-4.46320186	2.26401952	-0.28632999
C	-5.16351514	0.78012848	-0.12354201
C	-4.26112200	-0.37755300	-0.02007900
C	-6.54342000	0.20775500	-0.02985300
C	-6.60280700	-1.20765500	0.13419400
S	-4.98305300	-1.93670600	0.17419800
C	-7.82812800	-1.88148800	0.24301200
C	-8.20128900	-3.20616000	0.39636700
C	-9.56946100	-3.70021100	0.49137300
C	-9.49760900	-5.17774800	0.63683000
C	-8.14887300	-5.56438500	0.63180900
C	-7.29401600	-4.36437600	0.48450900
C	-10.48817000	-6.15302800	0.76607700
C	-10.08232000	-7.47382500	0.88453800
C	-8.73500200	-7.84068400	0.87742300

C	-7.74357300	-6.88321100	0.74995900
F	-11.00373800	-8.43950900	1.01049500
F	-8.41950000	-9.13773600	0.99636200
C	-10.75024000	-2.98164000	0.46000500
O	-6.07339600	-4.36695400	0.44510900
C	12.03141300	-3.59057600	-0.56430000
N	13.08558300	-4.05915200	-0.64686400
C	10.82096900	-1.56804600	-0.32169700
N	10.91010600	-0.41955600	-0.20969200
C	13.80662500	12.25104700	1.14466200
C	12.45709900	11.53399500	1.10546700
C	12.58630100	10.01751600	0.94361400
C	11.24162700	9.28874500	0.90249100
C	11.37398400	7.77298100	0.74019000
C	10.02989600	7.04309700	0.69642200
C	10.16560600	5.52788200	0.53302300
C	8.82249300	4.79667600	0.48534700
C	8.96507100	3.28287000	0.31984300
C	7.61869000	2.55622000	0.26767400
C	7.79635200	1.04759000	0.09584100
C	-13.80667700	12.25100900	-1.14461500
C	-12.45714600	11.53396200	-1.10543700
C	-12.58634100	10.01748400	-0.94357400
C	-11.24166400	9.28871800	-0.90246700
C	-11.37401100	7.77295500	-0.74015500
C	-10.02992100	7.04307600	-0.69640400
C	-10.16562300	5.52786100	-0.53299400
C	-8.82250800	4.79665900	-0.48533900
C	-8.96508200	3.28285400	-0.31982300
C	-7.61869900	2.55620400	-0.26767800
C	-7.79635800	1.04757600	-0.09583400
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C	-1.54668900	-1.89526500	0.51351900
C	2.26708100	-5.44755400	0.92369700
C	1.95736800	-4.36016700	-0.10315900
C	1.83929500	-2.97287900	0.53154800
C	1.54669000	-1.89523900	-0.51366000
H	6.69681300	-7.15947500	-0.74359700

H	11.54642900	-5.94094600	-0.77887100
H	8.65301100	-1.18757900	-0.19044200
H	-8.65300700	-1.18759900	0.19047000
H	-11.54639900	-5.94097200	0.77900800
H	-6.69677800	-7.15947900	0.74365500
H	13.68419500	13.33177500	1.26073100
H	14.37336500	12.07929300	0.22386400
H	14.41975300	11.89602800	1.97928900
H	11.85390800	11.93447900	0.28178200
H	11.90003000	11.75247100	2.02450100
H	13.14508800	9.79933500	0.02445500
H	13.19071600	9.61713700	1.76767700
H	10.63787700	9.68957800	0.07834900
H	10.68335300	9.50704500	1.82175900
H	11.93364800	7.55501700	-0.17821200
H	11.97666800	7.37198600	1.56491400
H	9.42712100	7.44378600	-0.12845700
H	9.46990200	7.25990200	1.61495200
H	10.72740700	5.31120300	-0.38414600
H	10.76662600	5.12658800	1.35856800
H	8.22111000	5.19733000	-0.34050400
H	8.26015100	5.01091300	1.40299400
H	9.52872100	3.06482200	-0.59475700
H	9.56283800	2.87777500	1.14472300
H	7.03162100	2.96073000	-0.56393500
H	7.06742500	2.76586200	1.19073600
H	8.42162700	0.67739400	0.91544700
H	8.38468400	0.86996400	-0.81069200
H	-14.41981600	11.89598300	-1.97923000
H	-14.37340000	12.07925900	-0.22380600
H	-13.68425300	13.33173700	-1.26069400
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H	-11.90009400	11.75243500	-2.02448100
H	-13.14511100	9.79930700	-0.02440500
H	-13.19076800	9.61709800	-1.76762300
H	-10.63790100	9.68955900	-0.07833700
H	-10.68340400	9.50701500	-1.82174500
H	-11.93366100	7.55499500	0.17825800
H	-11.97670800	7.37195300	-1.56486600
H	-9.42713500	7.44377100	0.12846200
H	-9.46994200	7.25987700	-1.61494500
H	-10.72740800	5.31118600	0.38418700
H	-10.76665800	5.12656100	-1.35852600
H	-8.22111200	5.19731800	0.34050000

H	-8.26018300	5.01089200	-1.40299600
H	-9.52871300	3.06481000	0.59478800
H	-9.56286400	2.87775400	-1.14469000
H	-7.03161400	2.96071900	0.56391900
H	-7.06745000	2.76584300	-1.19075100
H	-8.38466900	0.86995200	0.81071200
H	-8.42164900	0.67737700	-0.91542500
H	-2.33543000	-6.42946000	-0.44956000
H	-1.49210900	-5.50459900	-1.69503300
H	-3.22159600	-5.25318000	-1.42108000
H	-1.02903000	-4.60349500	0.63207900
H	-2.74976100	-4.34142500	0.85844700
H	-1.06502600	-2.97703500	-1.30467200
H	-2.77038500	-2.73395800	-1.05124300
H	-0.55536800	-2.00609200	0.94010200
H	-2.24750000	-1.99808700	1.34712900
H	1.49211100	-5.50476500	1.69459100
H	2.33549000	-6.42949900	0.44906100
H	3.22160100	-5.25328300	1.42070500
H	1.02907300	-4.60346800	-0.63245300
H	2.74980400	-4.34135100	-0.85876000
H	1.06499300	-2.97716500	1.30442800
H	2.77035500	-2.73404600	1.05107100
H	0.55537300	-2.00603600	-0.94025500
H	2.24750900	-1.99799600	-1.34727400

Y-S-Se-S(A2)

C	9.49763200	-5.17772900	-0.63675600
C	8.14889800	-5.56437200	-0.63175700
C	7.74360700	-6.88320200	-0.74988300
C	8.73504200	-7.84067300	-0.87730500
C	10.08235900	-7.47380800	-0.88440100
C	10.48820000	-6.15300700	-0.76596000
C	9.56947500	-3.70019000	-0.49131900
C	8.20130100	-3.20614300	-0.39634300
C	7.29403100	-4.36436000	-0.48451400
C	10.75025100	-2.98161600	-0.45992800
O	6.07341300	-4.36694700	-0.44510000
C	7.82813400	-1.88147200	-0.24300000
C	6.60281000	-1.20764100	-0.13420900
F	8.41954700	-9.13772900	-0.99622300
F	11.00378400	-8.43949300	-1.01031600
C	6.54341700	0.20776800	0.02983700
C	5.18905632	0.72600588	0.11757742

C	4.26111800	-0.37754800	0.02004700
C	2.77489000	1.45340900	0.21866200
C	2.92697200	0.06954200	0.09658300
C	1.40387200	1.73627600	0.16236000
C	0.71695900	0.48883800	0.03392600
N	1.67454000	-0.52245800	-0.01217200
C	0.71191100	2.98296800	0.11250700
C	-0.71192300	2.98296900	-0.11251100
C	-1.40388300	1.73627900	-0.16240100
C	-0.71696300	0.48883700	-0.03400200
N	1.24377500	4.19262900	0.19396800
S	-0.00000800	5.27431000	0.00003000
N	-1.24378700	4.19263200	-0.19394200
C	-2.77489900	1.45341000	-0.21870700
C	-2.92697800	0.06954200	-0.09662200
N	-1.67454600	-0.52245000	0.01213600
C	-5.16351514	0.78012848	-0.12354201
C	-4.26112200	-0.37755300	-0.02007900
C	-6.54342000	0.20775500	-0.02985300
C	-6.60280700	-1.20765500	0.13419400
C	-7.82812800	-1.88148800	0.24301200
C	-8.20128900	-3.20616000	0.39636700
C	-9.56946100	-3.70021100	0.49137300
C	-9.49760900	-5.17774800	0.63683000
C	-8.14887300	-5.56438500	0.63180900
C	-7.29401600	-4.36437600	0.48450900
C	-10.48817000	-6.15302800	0.76607700
C	-10.08232000	-7.47382500	0.88453800
C	-8.73500200	-7.84068400	0.87742300
C	-7.74357300	-6.88321100	0.74995900
F	-11.00373800	-8.43950900	1.01049500
F	-8.41950000	-9.13773600	0.99636200
C	-10.75024000	-2.98164000	0.46000500
O	-6.07339600	-4.36695400	0.44510900
C	12.03141300	-3.59057600	-0.56430000
N	13.08558300	-4.05915200	-0.64686400
C	10.82096900	-1.56804600	-0.32169700
N	10.91010600	-0.41955600	-0.20969200
C	13.80662500	12.25104700	1.14466200
C	12.45709900	11.53399500	1.10546700
C	12.58630100	10.01751600	0.94361400
C	11.24162700	9.28874500	0.90249100
C	11.37398400	7.77298100	0.74019000
C	10.02989600	7.04309700	0.69642200

C	10.16560600	5.52788200	0.53302300
C	8.82249300	4.79667600	0.48534700
C	8.96507100	3.28287000	0.31984300
C	7.61869000	2.55622000	0.26767400
C	7.79635200	1.04759000	0.09584100
C	-13.80667700	12.25100900	-1.14461500
C	-12.45714600	11.53396200	-1.10543700
C	-12.58634100	10.01748400	-0.94357400
C	-11.24166400	9.28871800	-0.90246700
C	-11.37401100	7.77295500	-0.74015500
C	-10.02992100	7.04307600	-0.69640400
C	-10.16562300	5.52786100	-0.53299400
C	-8.82250800	4.79665900	-0.48533900
C	-8.96508200	3.28285400	-0.31982300
C	-7.61869900	2.55620400	-0.26767800
C	-7.79635800	1.04757600	-0.09583400
C	-12.03139700	-3.59060000	0.56441200
N	-13.08557000	-4.05916300	0.64700600
C	-10.82096100	-1.56807100	0.32176300
N	-10.91011300	-0.41958300	0.20974100
C	-2.26705800	-5.44747300	-0.92411300
C	-1.95734100	-4.36016500	0.10282600
C	-1.83930500	-2.97282400	-0.53176900
C	-1.54668900	-1.89526500	0.51351900
C	2.26708100	-5.44755400	0.92369700
C	1.95736800	-4.36016700	-0.10315900
C	1.83929500	-2.97287900	0.53154800
C	1.54669000	-1.89523900	-0.51366000
H	6.69681300	-7.15947500	-0.74359700
H	11.54642900	-5.94094600	-0.77887100
H	8.65301100	-1.18757900	-0.19044200
H	-8.65300700	-1.18759900	0.19047000
H	-11.54639900	-5.94097200	0.77900800
H	-6.69677800	-7.15947900	0.74365500
H	13.68419500	13.33177500	1.26073100
H	14.37336500	12.07929300	0.22386400
H	14.41975300	11.89602800	1.97928900
H	11.85390800	11.93447900	0.28178200
H	11.90003000	11.75247100	2.02450100
H	13.14508800	9.79933500	0.02445500
H	13.19071600	9.61713700	1.76767700
H	10.63787700	9.68957800	0.07834900
H	10.68335300	9.50704500	1.82175900
H	11.93364800	7.55501700	-0.17821200

H	11.97666800	7.37198600	1.56491400
H	9.42712100	7.44378600	-0.12845700
H	9.46990200	7.25990200	1.61495200
H	10.72740700	5.31120300	-0.38414600
H	10.76662600	5.12658800	1.35856800
H	8.22111000	5.19733000	-0.34050400
H	8.26015100	5.01091300	1.40299400
H	9.52872100	3.06482200	-0.59475700
H	9.56283800	2.87777500	1.14472300
H	7.03162100	2.96073000	-0.56393500
H	7.06742500	2.76586200	1.19073600
H	8.42162700	0.67739400	0.91544700
H	8.38468400	0.86996400	-0.81069200
H	-14.41981600	11.89598300	-1.97923000
H	-14.37340000	12.07925900	-0.22380600
H	-13.68425300	13.33173700	-1.26069400
H	-11.85394400	11.93445400	-0.28176500
H	-11.90009400	11.75243500	-2.02448100
H	-13.14511100	9.79930700	-0.02440500
H	-13.19076800	9.61709800	-1.76762300
H	-10.63790100	9.68955900	-0.07833700
H	-10.68340400	9.50701500	-1.82174500
H	-11.93366100	7.55499500	0.17825800
H	-11.97670800	7.37195300	-1.56486600
H	-9.42713500	7.44377100	0.12846200
H	-9.46994200	7.25987700	-1.61494500
H	-10.72740800	5.31118600	0.38418700
H	-10.76665800	5.12656100	-1.35852600
H	-8.22111200	5.19731800	0.34050000
H	-8.26018300	5.01089200	-1.40299600
H	-9.52871300	3.06481000	0.59478800
H	-9.56286400	2.87775400	-1.14469000
H	-7.03161400	2.96071900	0.56391900
H	-7.06745000	2.76584300	-1.19075100
H	-8.38466900	0.86995200	0.81071200
H	-8.42164900	0.67737700	-0.91542500
H	-2.33543000	-6.42946000	-0.44956000
H	-1.49210900	-5.50459900	-1.69503300
H	-3.22159600	-5.25318000	-1.42108000
H	-1.02903000	-4.60349500	0.63207900
H	-2.74976100	-4.34142500	0.85844700
H	-1.06502600	-2.97703500	-1.30467200
H	-2.77038500	-2.73395800	-1.05124300
H	-0.55536800	-2.00609200	0.94010200

H	-2.24750000	-1.99808700	1.34712900
H	1.49211100	-5.50476500	1.69459100
H	2.33549000	-6.42949900	0.44906100
H	3.22160100	-5.25328300	1.42070500
H	1.02907300	-4.60346800	-0.63245300
H	2.74980400	-4.34135100	-0.85876000
H	1.06499300	-2.97716500	1.30442800
H	2.77035500	-2.73404600	1.05107100
H	0.55537300	-2.00603600	-0.94025500
H	2.24750900	-1.99799600	-1.34727400
Se	-4.46320186	2.26401952	-0.28632999
Se	4.43764168	2.31815512	0.29223558
S	-4.98305300	-1.93670600	0.17419800
S	4.98305900	-1.93669500	-0.17424700

Y-S-S-Se(A3)

C	-9.86122900	-4.91941100	0.70047100
C	-8.53498700	-5.38698500	0.74153000
C	-8.21079200	-6.72494600	0.91119500
C	-9.26260500	-7.61946600	1.04387000
C	-10.58900100	-7.17125400	1.00539300
C	-10.91285200	-5.83041700	0.83527600
C	-9.83754100	-3.44545800	0.50745000
C	-8.43870800	-3.04119100	0.43133000
C	-7.61147900	-4.24506700	0.57725900
C	-10.96765000	-2.64966200	0.42156600
O	-6.38196100	-4.31933000	0.57329100
C	-7.96765500	-1.74911200	0.25557700
C	-6.68378300	-1.19736400	0.15562900
F	-9.03539400	-8.92746000	1.21093500
F	-11.56406200	-8.07866900	1.13843200
C	-6.50016500	0.20535800	-0.02186100
C	-5.14791200	0.57258800	-0.09726600
C	-4.21876600	-0.49134800	-0.00331600
S	-4.33443600	2.15715600	-0.27850300
C	-2.78816800	1.35847600	-0.20446600
C	-2.89798300	-0.03129500	-0.07868600
C	-1.41824600	1.68015600	-0.15058600
C	-0.71295100	0.44415000	-0.02104400
N	-1.63522200	-0.59705800	0.03141600
C	-0.71731900	2.92660500	-0.10603600
C	0.71707700	2.92666400	0.10421300
C	1.41804900	1.68025000	0.14913500
C	0.71279900	0.44418700	0.02000500

N	-1.25102200	4.13824300	-0.18402900
S	-0.00016300	5.21683700	-0.00127500
N	1.25073700	4.13834500	0.18180600
C	2.78798200	1.35862500	0.20320400
C	2.89784700	-0.03118000	0.07789700
N	1.63509300	-0.59704500	-0.03201200
S	4.33421200	2.15739700	0.27706900
C	5.14777200	0.57276800	0.09636600
C	4.21864800	-0.49121200	0.00273000
C	6.50003300	0.20555600	0.02114300
C	6.68370600	-1.19720300	-0.15594700
C	7.96761700	-1.74888800	-0.25574300
C	8.43884100	-3.04096100	-0.43115700
C	9.83773200	-3.44507000	-0.50706700
C	9.86163100	-4.91904400	-0.69986900
C	8.53545900	-5.38680400	-0.74093800
C	7.61179000	-4.24498900	-0.57688100
C	10.91339100	-5.82992100	-0.83449100
C	10.58973600	-7.17082500	-1.00444400
C	9.26340400	-7.61922600	-1.04293000
C	8.21145900	-6.72483300	-0.91044100
F	11.56493000	-8.07812200	-1.13731500
F	9.03638300	-8.92727600	-1.20982200
C	10.96775200	-2.64914600	-0.42115300
O	6.38228000	-4.31943900	-0.57301100
C	-12.29095400	-3.17247800	0.51146800
N	-13.37910700	-3.58131300	0.58266500
C	-10.93297000	-1.23626600	0.23618800
N	-10.92791100	-0.08053200	0.08535000
C	-13.05337300	12.62807000	-1.50283300
C	-11.75097900	11.83233200	-1.41423000
C	-11.97585300	10.33020500	-1.22013600
C	-10.67725300	9.52469400	-1.13122700
C	-10.90178300	8.02291900	-0.93692700
C	-9.60173100	7.21931000	-0.85072000
C	-9.82410700	5.71738600	-0.65575300
C	-8.52166800	4.91735200	-0.57390500
C	-8.74327100	3.41607600	-0.37779700
C	-7.43387000	2.62447300	-0.30239000
C	-7.69536300	1.13089400	-0.10338000
C	13.05277100	12.62818500	1.50484900
C	11.75041400	11.83238900	1.41622800
C	11.97535200	10.33035100	1.22152200
C	10.67678800	9.52478400	1.13258500

C	10.90137900	8.02309700	0.93767200
C	9.60136300	7.21943400	0.85144100
C	9.82379500	5.71759800	0.65586600
C	8.52138900	4.91751100	0.57399800
C	8.74304100	3.41631900	0.37731000
C	7.43367000	2.62467100	0.30188800
C	7.69519600	1.13116600	0.10234900
C	12.29111200	-3.17185400	-0.51085000
N	13.37930800	-3.58060000	-0.58188400
C	10.93292300	-1.23573700	-0.23591300
N	10.92780100	-0.07999000	-0.08517900
C	3.10536400	-5.29728800	0.40380600
C	2.40550600	-4.30208000	-0.52119500
C	1.89076700	-3.07716900	0.24739800
C	1.49220600	-1.91370500	-0.67129100
C	-3.10494600	-5.29759700	-0.40371600
C	-2.40545000	-4.30199300	0.52113700
C	-1.89068100	-3.07723600	-0.24767900
C	-1.49225500	-1.91360800	0.67085200
H	-7.18069200	-7.06096600	0.93900900
H	-11.95744500	-5.55344200	0.81483700
H	-8.73701300	-0.99523300	0.17867400
H	8.73690000	-0.99491200	-0.17905100
H	11.95794300	-5.55279000	-0.81404100
H	7.18140700	-7.06100200	-0.93826200
H	-12.86344900	13.69759700	-1.64140400
H	-13.65143700	12.51319500	-0.59149100
H	-13.66897500	12.28922900	-2.34404300
H	-11.14177600	12.21672100	-0.58510800
H	-11.15923300	11.99445400	-2.32521200
H	-12.56815600	10.16764200	-0.30854700
H	-12.58659100	9.94551200	-2.04914300
H	-10.06688500	9.91040400	-0.30256100
H	-10.08581500	9.68797000	-2.04312900
H	-11.49148100	7.85883400	-0.02415800
H	-11.51294900	7.63688100	-1.76473500
H	-8.99010900	7.60597500	-0.02348600
H	-9.01260300	7.38329400	-1.76393700
H	-10.41024400	5.55174400	0.25882000
H	-10.43680100	5.32980000	-1.48147700
H	-7.90793200	5.30520400	0.25107100
H	-7.93608100	5.08194600	-1.48917000
H	-9.32420400	3.24519100	0.53823800
H	-9.35792600	3.02318100	-1.19853500

H	-6.82805900	3.01514900	0.52371900
H	-6.86414500	2.78815700	-1.22475800
H	-8.34581400	0.78604500	-0.91664800
H	-8.29569100	1.00541300	0.80623200
H	13.66857700	12.28907400	2.34580100
H	13.65064800	12.51369200	0.59333600
H	12.86280200	13.69764800	1.64385900
H	11.14100700	12.21704600	0.58737900
H	11.15885200	11.99412800	2.32739600
H	12.56747200	10.16817200	0.30974600
H	12.58629200	9.94538900	2.05025500
H	10.06621700	9.91076400	0.30419500
H	10.08553400	9.68767600	2.04467500
H	11.49089400	7.85939500	0.02471600
H	11.51274700	7.63679000	1.76520500
H	8.98953800	7.60636800	0.02448200
H	9.01241900	7.38303700	1.76484500
H	10.40974800	5.55233300	-0.25889400
H	10.43668900	5.32974300	1.48131500
H	7.90745600	5.30562400	-0.25071000
H	7.93598200	5.08174000	1.48944400
H	9.32379800	3.24579700	-0.53890500
H	9.35788500	3.02316600	1.19778300
H	6.82770400	3.01560300	-0.52398600
H	6.86409100	2.78801000	1.22440700
H	8.29512500	1.00594400	-0.80757400
H	8.34604600	0.78618600	0.91523000
H	3.45868500	-6.17236600	-0.14884800
H	2.44066700	-5.64661200	1.20174900
H	3.97780600	-4.82328400	0.86488200
H	1.57963900	-4.78425600	-1.05900700
H	3.12217700	-3.97372400	-1.28466500
H	1.05453500	-3.36677500	0.89340700
H	2.67657900	-2.73321200	0.92914000
H	0.47413300	-2.00365500	-1.04495100
H	2.14532400	-1.90789700	-1.55168600
H	-2.43996300	-5.64705700	-1.20136000
H	-3.45826800	-6.17256900	0.14911500
H	-3.97733900	-4.82389200	-0.86518800
H	-1.57963300	-4.78392500	1.05925500
H	-3.12232300	-3.97350000	1.28434700
H	-1.05436600	-3.36694100	-0.89353600
H	-2.67643000	-2.73343500	-0.92955600
H	-0.47420900	-2.00343400	1.04458300

H	-2.14542000	-1.90772000	1.55121500
Se	5.03044600	-2.15114200	-0.21425400
Se	-5.03048800	-2.15123400	0.21420500

Y-S-Se-Se(A4)

C	9.49763200	-5.17772900	-0.63675600
C	8.14889800	-5.56437200	-0.63175700
C	7.74360700	-6.88320200	-0.74988300
C	8.73504200	-7.84067300	-0.87730500
C	10.08235900	-7.47380800	-0.88440100
C	10.48820000	-6.15300700	-0.76596000
C	9.56947500	-3.70019000	-0.49131900
C	8.20130100	-3.20614300	-0.39634300
C	7.29403100	-4.36436000	-0.48451400
C	10.75025100	-2.98161600	-0.45992800
O	6.07341300	-4.36694700	-0.44510000
C	7.82813400	-1.88147200	-0.24300000
C	6.60281000	-1.20764100	-0.13420900
F	8.41954700	-9.13772900	-0.99622300
F	11.00378400	-8.43949300	-1.01031600
C	6.54341700	0.20776800	0.02983700
C	5.18905632	0.72600588	0.11757742
C	4.26111800	-0.37754800	0.02004700
C	2.77489000	1.45340900	0.21866200
C	2.92697200	0.06954200	0.09658300
C	1.40387200	1.73627600	0.16236000
C	0.71695900	0.48883800	0.03392600
N	1.67454000	-0.52245800	-0.01217200
C	0.71191100	2.98296800	0.11250700
C	-0.71192300	2.98296900	-0.11251100
C	-1.40388300	1.73627900	-0.16240100
C	-0.71696300	0.48883700	-0.03400200
N	1.24377500	4.19262900	0.19396800
S	-0.00000800	5.27431000	0.00003000
N	-1.24378700	4.19263200	-0.19394200
C	-2.77489900	1.45341000	-0.21870700
C	-2.92697800	0.06954200	-0.09662200
N	-1.67454600	-0.52245000	0.01213600
C	-5.16351514	0.78012848	-0.12354201
C	-4.26112200	-0.37755300	-0.02007900
C	-6.54342000	0.20775500	-0.02985300
C	-6.60280700	-1.20765500	0.13419400
C	-7.82812800	-1.88148800	0.24301200
C	-8.20128900	-3.20616000	0.39636700

C	-9.56946100	-3.70021100	0.49137300
C	-9.49760900	-5.17774800	0.63683000
C	-8.14887300	-5.56438500	0.63180900
C	-7.29401600	-4.36437600	0.48450900
C	-10.48817000	-6.15302800	0.76607700
C	-10.08232000	-7.47382500	0.88453800
C	-8.73500200	-7.84068400	0.87742300
C	-7.74357300	-6.88321100	0.74995900
F	-11.00373800	-8.43950900	1.01049500
F	-8.41950000	-9.13773600	0.99636200
C	-10.75024000	-2.98164000	0.46000500
O	-6.07339600	-4.36695400	0.44510900
C	12.03141300	-3.59057600	-0.56430000
N	13.08558300	-4.05915200	-0.64686400
C	10.82096900	-1.56804600	-0.32169700
N	10.91010600	-0.41955600	-0.20969200
C	13.80662500	12.25104700	1.14466200
C	12.45709900	11.53399500	1.10546700
C	12.58630100	10.01751600	0.94361400
C	11.24162700	9.28874500	0.90249100
C	11.37398400	7.77298100	0.74019000
C	10.02989600	7.04309700	0.69642200
C	10.16560600	5.52788200	0.53302300
C	8.82249300	4.79667600	0.48534700
C	8.96507100	3.28287000	0.31984300
C	7.61869000	2.55622000	0.26767400
C	7.79635200	1.04759000	0.09584100
C	-13.80667700	12.25100900	-1.14461500
C	-12.45714600	11.53396200	-1.10543700
C	-12.58634100	10.01748400	-0.94357400
C	-11.24166400	9.28871800	-0.90246700
C	-11.37401100	7.77295500	-0.74015500
C	-10.02992100	7.04307600	-0.69640400
C	-10.16562300	5.52786100	-0.53299400
C	-8.82250800	4.79665900	-0.48533900
C	-8.96508200	3.28285400	-0.31982300
C	-7.61869900	2.55620400	-0.26767800
C	-7.79635800	1.04757600	-0.09583400
C	-12.03139700	-3.59060000	0.56441200
N	-13.08557000	-4.05916300	0.64700600
C	-10.82096100	-1.56807100	0.32176300
N	-10.91011300	-0.41958300	0.20974100
C	-2.26705800	-5.44747300	-0.92411300
C	-1.95734100	-4.36016500	0.10282600

C	-1.83930500	-2.97282400	-0.53176900
C	-1.54668900	-1.89526500	0.51351900
C	2.26708100	-5.44755400	0.92369700
C	1.95736800	-4.36016700	-0.10315900
C	1.83929500	-2.97287900	0.53154800
C	1.54669000	-1.89523900	-0.51366000
H	6.69681300	-7.15947500	-0.74359700
H	11.54642900	-5.94094600	-0.77887100
H	8.65301100	-1.18757900	-0.19044200
H	-8.65300700	-1.18759900	0.19047000
H	-11.54639900	-5.94097200	0.77900800
H	-6.69677800	-7.15947900	0.74365500
H	13.68419500	13.33177500	1.26073100
H	14.37336500	12.07929300	0.22386400
H	14.41975300	11.89602800	1.97928900
H	11.85390800	11.93447900	0.28178200
H	11.90003000	11.75247100	2.02450100
H	13.14508800	9.79933500	0.02445500
H	13.19071600	9.61713700	1.76767700
H	10.63787700	9.68957800	0.07834900
H	10.68335300	9.50704500	1.82175900
H	11.93364800	7.55501700	-0.17821200
H	11.97666800	7.37198600	1.56491400
H	9.42712100	7.44378600	-0.12845700
H	9.46990200	7.25990200	1.61495200
H	10.72740700	5.31120300	-0.38414600
H	10.76662600	5.12658800	1.35856800
H	8.22111000	5.19733000	-0.34050400
H	8.26015100	5.01091300	1.40299400
H	9.52872100	3.06482200	-0.59475700
H	9.56283800	2.87777500	1.14472300
H	7.03162100	2.96073000	-0.56393500
H	7.06742500	2.76586200	1.19073600
H	8.42162700	0.67739400	0.91544700
H	8.38468400	0.86996400	-0.81069200
H	-14.41981600	11.89598300	-1.97923000
H	-14.37340000	12.07925900	-0.22380600
H	-13.68425300	13.33173700	-1.26069400
H	-11.85394400	11.93445400	-0.28176500
H	-11.90009400	11.75243500	-2.02448100
H	-13.14511100	9.79930700	-0.02440500
H	-13.19076800	9.61709800	-1.76762300
H	-10.63790100	9.68955900	-0.07833700
H	-10.68340400	9.50701500	-1.82174500

H	-11.93366100	7.55499500	0.17825800
H	-11.97670800	7.37195300	-1.56486600
H	-9.42713500	7.44377100	0.12846200
H	-9.46994200	7.25987700	-1.61494500
H	-10.72740800	5.31118600	0.38418700
H	-10.76665800	5.12656100	-1.35852600
H	-8.22111200	5.19731800	0.34050000
H	-8.26018300	5.01089200	-1.40299600
H	-9.52871300	3.06481000	0.59478800
H	-9.56286400	2.87775400	-1.14469000
H	-7.03161400	2.96071900	0.56391900
H	-7.06745000	2.76584300	-1.19075100
H	-8.38466900	0.86995200	0.81071200
H	-8.42164900	0.67737700	-0.91542500
H	-2.33543000	-6.42946000	-0.44956000
H	-1.49210900	-5.50459900	-1.69503300
H	-3.22159600	-5.25318000	-1.42108000
H	-1.02903000	-4.60349500	0.63207900
H	-2.74976100	-4.34142500	0.85844700
H	-1.06502600	-2.97703500	-1.30467200
H	-2.77038500	-2.73395800	-1.05124300
H	-0.55536800	-2.00609200	0.94010200
H	-2.24750000	-1.99808700	1.34712900
H	1.49211100	-5.50476500	1.69459100
H	2.33549000	-6.42949900	0.44906100
H	3.22160100	-5.25328300	1.42070500
H	1.02907300	-4.60346800	-0.63245300
H	2.74980400	-4.34135100	-0.85876000
H	1.06499300	-2.97716500	1.30442800
H	2.77035500	-2.73404600	1.05107100
H	0.55537300	-2.00603600	-0.94025500
H	2.24750900	-1.99799600	-1.34727400
Se	-4.46320186	2.26401952	-0.28632999
Se	4.43764168	2.31815512	0.29223558
Se	-4.98305300	-1.93670600	0.17419800
Se	4.98305900	-1.93669500	-0.17424700

Y6-Se(B1)

C	9.49763200	-5.17772900	-0.63675600
C	8.14889800	-5.56437200	-0.63175700
C	7.74360700	-6.88320200	-0.74988300
C	8.73504200	-7.84067300	-0.87730500
C	10.08235900	-7.47380800	-0.88440100
C	10.48820000	-6.15300700	-0.76596000

C	9.56947500	-3.70019000	-0.49131900
C	8.20130100	-3.20614300	-0.39634300
C	7.29403100	-4.36436000	-0.48451400
C	10.75025100	-2.98161600	-0.45992800
O	6.07341300	-4.36694700	-0.44510000
C	7.82813400	-1.88147200	-0.24300000
C	6.60281000	-1.20764100	-0.13420900
F	8.41954700	-9.13772900	-0.99622300
F	11.00378400	-8.43949300	-1.01031600
C	6.54341700	0.20776800	0.02983700
C	5.18905632	0.72600588	0.11757742
C	4.26111800	-0.37754800	0.02004700
C	2.77489000	1.45340900	0.21866200
C	2.92697200	0.06954200	0.09658300
C	1.40387200	1.73627600	0.16236000
C	0.71695900	0.48883800	0.03392600
N	1.67454000	-0.52245800	-0.01217200
C	0.71191100	2.98296800	0.11250700
C	-0.71192300	2.98296900	-0.11251100
C	-1.40388300	1.73627900	-0.16240100
C	-0.71696300	0.48883700	-0.03400200
N	1.24377500	4.19262900	0.19396800
N	-1.24378700	4.19263200	-0.19394200
C	-2.77489900	1.45341000	-0.21870700
C	-2.92697800	0.06954200	-0.09662200
N	-1.67454600	-0.52245000	0.01213600
C	-5.16351514	0.78012848	-0.12354201
C	-4.26112200	-0.37755300	-0.02007900
C	-6.54342000	0.20775500	-0.02985300
C	-6.60280700	-1.20765500	0.13419400
C	-7.82812800	-1.88148800	0.24301200
C	-8.20128900	-3.20616000	0.39636700
C	-9.56946100	-3.70021100	0.49137300
C	-9.49760900	-5.17774800	0.63683000
C	-8.14887300	-5.56438500	0.63180900
C	-7.29401600	-4.36437600	0.48450900
C	-10.48817000	-6.15302800	0.76607700
C	-10.08232000	-7.47382500	0.88453800
C	-8.73500200	-7.84068400	0.87742300
C	-7.74357300	-6.88321100	0.74995900
F	-11.00373800	-8.43950900	1.01049500
F	-8.41950000	-9.13773600	0.99636200
C	-10.75024000	-2.98164000	0.46000500
O	-6.07339600	-4.36695400	0.44510900

C	12.03141300	-3.59057600	-0.56430000
N	13.08558300	-4.05915200	-0.64686400
C	10.82096900	-1.56804600	-0.32169700
N	10.91010600	-0.41955600	-0.20969200
C	13.80662500	12.25104700	1.14466200
C	12.45709900	11.53399500	1.10546700
C	12.58630100	10.01751600	0.94361400
C	11.24162700	9.28874500	0.90249100
C	11.37398400	7.77298100	0.74019000
C	10.02989600	7.04309700	0.69642200
C	10.16560600	5.52788200	0.53302300
C	8.82249300	4.79667600	0.48534700
C	8.96507100	3.28287000	0.31984300
C	7.61869000	2.55622000	0.26767400
C	7.79635200	1.04759000	0.09584100
C	-13.80667700	12.25100900	-1.14461500
C	-12.45714600	11.53396200	-1.10543700
C	-12.58634100	10.01748400	-0.94357400
C	-11.24166400	9.28871800	-0.90246700
C	-11.37401100	7.77295500	-0.74015500
C	-10.02992100	7.04307600	-0.69640400
C	-10.16562300	5.52786100	-0.53299400
C	-8.82250800	4.79665900	-0.48533900
C	-8.96508200	3.28285400	-0.31982300
C	-7.61869900	2.55620400	-0.26767800
C	-7.79635800	1.04757600	-0.09583400
C	-12.03139700	-3.59060000	0.56441200
N	-13.08557000	-4.05916300	0.64700600
C	-10.82096100	-1.56807100	0.32176300
N	-10.91011300	-0.41958300	0.20974100
C	-2.26705800	-5.44747300	-0.92411300
C	-1.95734100	-4.36016500	0.10282600
C	-1.83930500	-2.97282400	-0.53176900
C	-1.54668900	-1.89526500	0.51351900
C	2.26708100	-5.44755400	0.92369700
C	1.95736800	-4.36016700	-0.10315900
C	1.83929500	-2.97287900	0.53154800
C	1.54669000	-1.89523900	-0.51366000
H	6.69681300	-7.15947500	-0.74359700
H	11.54642900	-5.94094600	-0.77887100
H	8.65301100	-1.18757900	-0.19044200
H	-8.65300700	-1.18759900	0.19047000
H	-11.54639900	-5.94097200	0.77900800
H	-6.69677800	-7.15947900	0.74365500

H	13.68419500	13.33177500	1.26073100
H	14.37336500	12.07929300	0.22386400
H	14.41975300	11.89602800	1.97928900
H	11.85390800	11.93447900	0.28178200
H	11.90003000	11.75247100	2.02450100
H	13.14508800	9.79933500	0.02445500
H	13.19071600	9.61713700	1.76767700
H	10.63787700	9.68957800	0.07834900
H	10.68335300	9.50704500	1.82175900
H	11.93364800	7.55501700	-0.17821200
H	11.97666800	7.37198600	1.56491400
H	9.42712100	7.44378600	-0.12845700
H	9.46990200	7.25990200	1.61495200
H	10.72740700	5.31120300	-0.38414600
H	10.76662600	5.12658800	1.35856800
H	8.22111000	5.19733000	-0.34050400
H	8.26015100	5.01091300	1.40299400
H	9.52872100	3.06482200	-0.59475700
H	9.56283800	2.87777500	1.14472300
H	7.03162100	2.96073000	-0.56393500
H	7.06742500	2.76586200	1.19073600
H	8.42162700	0.67739400	0.91544700
H	8.38468400	0.86996400	-0.81069200
H	-14.41981600	11.89598300	-1.97923000
H	-14.37340000	12.07925900	-0.22380600
H	-13.68425300	13.33173700	-1.26069400
H	-11.85394400	11.93445400	-0.28176500
H	-11.90009400	11.75243500	-2.02448100
H	-13.14511100	9.79930700	-0.02440500
H	-13.19076800	9.61709800	-1.76762300
H	-10.63790100	9.68955900	-0.07833700
H	-10.68340400	9.50701500	-1.82174500
H	-11.93366100	7.55499500	0.17825800
H	-11.97670800	7.37195300	-1.56486600
H	-9.42713500	7.44377100	0.12846200
H	-9.46994200	7.25987700	-1.61494500
H	-10.72740800	5.31118600	0.38418700
H	-10.76665800	5.12656100	-1.35852600
H	-8.22111200	5.19731800	0.34050000
H	-8.26018300	5.01089200	-1.40299600
H	-9.52871300	3.06481000	0.59478800
H	-9.56286400	2.87775400	-1.14469000
H	-7.03161400	2.96071900	0.56391900
H	-7.06745000	2.76584300	-1.19075100

H	-8.38466900	0.86995200	0.81071200
H	-8.42164900	0.67737700	-0.91542500
H	-2.33543000	-6.42946000	-0.44956000
H	-1.49210900	-5.50459900	-1.69503300
H	-3.22159600	-5.25318000	-1.42108000
H	-1.02903000	-4.60349500	0.63207900
H	-2.74976100	-4.34142500	0.85844700
H	-1.06502600	-2.97703500	-1.30467200
H	-2.77038500	-2.73395800	-1.05124300
H	-0.55536800	-2.00609200	0.94010200
H	-2.24750000	-1.99808700	1.34712900
H	1.49211100	-5.50476500	1.69459100
H	2.33549000	-6.42949900	0.44906100
H	3.22160100	-5.25328300	1.42070500
H	1.02907300	-4.60346800	-0.63245300
H	2.74980400	-4.34135100	-0.85876000
H	1.06499300	-2.97716500	1.30442800
H	2.77035500	-2.73404600	1.05107100
H	0.55537300	-2.00603600	-0.94025500
H	2.24750900	-1.99799600	-1.34727400
Se	-0.00000800	5.27431000	0.00003000
S	-4.98305300	-1.93670600	0.17419800
S	4.98305900	-1.93669500	-0.17424700
S	-4.46320186	2.26401952	-0.28632999
S	4.43764168	2.31815512	0.29223558

Y6-Se-Se-S(B2)

C	9.49763200	-5.17772900	-0.63675600
C	8.14889800	-5.56437200	-0.63175700
C	7.74360700	-6.88320200	-0.74988300
C	8.73504200	-7.84067300	-0.87730500
C	10.08235900	-7.47380800	-0.88440100
C	10.48820000	-6.15300700	-0.76596000
C	9.56947500	-3.70019000	-0.49131900
C	8.20130100	-3.20614300	-0.39634300
C	7.29403100	-4.36436000	-0.48451400
C	10.75025100	-2.98161600	-0.45992800
O	6.07341300	-4.36694700	-0.44510000
C	7.82813400	-1.88147200	-0.24300000
C	6.60281000	-1.20764100	-0.13420900
F	8.41954700	-9.13772900	-0.99622300
F	11.00378400	-8.43949300	-1.01031600
C	6.54341700	0.20776800	0.02983700
C	5.18905632	0.72600588	0.11757742

C	4.26111800	-0.37754800	0.02004700
C	2.77489000	1.45340900	0.21866200
C	2.92697200	0.06954200	0.09658300
C	1.40387200	1.73627600	0.16236000
C	0.71695900	0.48883800	0.03392600
N	1.67454000	-0.52245800	-0.01217200
C	0.71191100	2.98296800	0.11250700
C	-0.71192300	2.98296900	-0.11251100
C	-1.40388300	1.73627900	-0.16240100
C	-0.71696300	0.48883700	-0.03400200
N	1.24377500	4.19262900	0.19396800
N	-1.24378700	4.19263200	-0.19394200
C	-2.77489900	1.45341000	-0.21870700
C	-2.92697800	0.06954200	-0.09662200
N	-1.67454600	-0.52245000	0.01213600
C	-5.16351514	0.78012848	-0.12354201
C	-4.26112200	-0.37755300	-0.02007900
C	-6.54342000	0.20775500	-0.02985300
C	-6.60280700	-1.20765500	0.13419400
C	-7.82812800	-1.88148800	0.24301200
C	-8.20128900	-3.20616000	0.39636700
C	-9.56946100	-3.70021100	0.49137300
C	-9.49760900	-5.17774800	0.63683000
C	-8.14887300	-5.56438500	0.63180900
C	-7.29401600	-4.36437600	0.48450900
C	-10.48817000	-6.15302800	0.76607700
C	-10.08232000	-7.47382500	0.88453800
C	-8.73500200	-7.84068400	0.87742300
C	-7.74357300	-6.88321100	0.74995900
F	-11.00373800	-8.43950900	1.01049500
F	-8.41950000	-9.13773600	0.99636200
C	-10.75024000	-2.98164000	0.46000500
O	-6.07339600	-4.36695400	0.44510900
C	12.03141300	-3.59057600	-0.56430000
N	13.08558300	-4.05915200	-0.64686400
C	10.82096900	-1.56804600	-0.32169700
N	10.91010600	-0.41955600	-0.20969200
C	13.80662500	12.25104700	1.14466200
C	12.45709900	11.53399500	1.10546700
C	12.58630100	10.01751600	0.94361400
C	11.24162700	9.28874500	0.90249100
C	11.37398400	7.77298100	0.74019000
C	10.02989600	7.04309700	0.69642200
C	10.16560600	5.52788200	0.53302300

C	8.82249300	4.79667600	0.48534700
C	8.96507100	3.28287000	0.31984300
C	7.61869000	2.55622000	0.26767400
C	7.79635200	1.04759000	0.09584100
C	-13.80667700	12.25100900	-1.14461500
C	-12.45714600	11.53396200	-1.10543700
C	-12.58634100	10.01748400	-0.94357400
C	-11.24166400	9.28871800	-0.90246700
C	-11.37401100	7.77295500	-0.74015500
C	-10.02992100	7.04307600	-0.69640400
C	-10.16562300	5.52786100	-0.53299400
C	-8.82250800	4.79665900	-0.48533900
C	-8.96508200	3.28285400	-0.31982300
C	-7.61869900	2.55620400	-0.26767800
C	-7.79635800	1.04757600	-0.09583400
C	-12.03139700	-3.59060000	0.56441200
N	-13.08557000	-4.05916300	0.64700600
C	-10.82096100	-1.56807100	0.32176300
N	-10.91011300	-0.41958300	0.20974100
C	-2.26705800	-5.44747300	-0.92411300
C	-1.95734100	-4.36016500	0.10282600
C	-1.83930500	-2.97282400	-0.53176900
C	-1.54668900	-1.89526500	0.51351900
C	2.26708100	-5.44755400	0.92369700
C	1.95736800	-4.36016700	-0.10315900
C	1.83929500	-2.97287900	0.53154800
C	1.54669000	-1.89523900	-0.51366000
H	6.69681300	-7.15947500	-0.74359700
H	11.54642900	-5.94094600	-0.77887100
H	8.65301100	-1.18757900	-0.19044200
H	-8.65300700	-1.18759900	0.19047000
H	-11.54639900	-5.94097200	0.77900800
H	-6.69677800	-7.15947900	0.74365500
H	13.68419500	13.33177500	1.26073100
H	14.37336500	12.07929300	0.22386400
H	14.41975300	11.89602800	1.97928900
H	11.85390800	11.93447900	0.28178200
H	11.90003000	11.75247100	2.02450100
H	13.14508800	9.79933500	0.02445500
H	13.19071600	9.61713700	1.76767700
H	10.63787700	9.68957800	0.07834900
H	10.68335300	9.50704500	1.82175900
H	11.93364800	7.55501700	-0.17821200
H	11.97666800	7.37198600	1.56491400

H	9.42712100	7.44378600	-0.12845700
H	9.46990200	7.25990200	1.61495200
H	10.72740700	5.31120300	-0.38414600
H	10.76662600	5.12658800	1.35856800
H	8.22111000	5.19733000	-0.34050400
H	8.26015100	5.01091300	1.40299400
H	9.52872100	3.06482200	-0.59475700
H	9.56283800	2.87777500	1.14472300
H	7.03162100	2.96073000	-0.56393500
H	7.06742500	2.76586200	1.19073600
H	8.42162700	0.67739400	0.91544700
H	8.38468400	0.86996400	-0.81069200
H	-14.41981600	11.89598300	-1.97923000
H	-14.37340000	12.07925900	-0.22380600
H	-13.68425300	13.33173700	-1.26069400
H	-11.85394400	11.93445400	-0.28176500
H	-11.90009400	11.75243500	-2.02448100
H	-13.14511100	9.79930700	-0.02440500
H	-13.19076800	9.61709800	-1.76762300
H	-10.63790100	9.68955900	-0.07833700
H	-10.68340400	9.50701500	-1.82174500
H	-11.93366100	7.55499500	0.17825800
H	-11.97670800	7.37195300	-1.56486600
H	-9.42713500	7.44377100	0.12846200
H	-9.46994200	7.25987700	-1.61494500
H	-10.72740800	5.31118600	0.38418700
H	-10.76665800	5.12656100	-1.35852600
H	-8.22111200	5.19731800	0.34050000
H	-8.26018300	5.01089200	-1.40299600
H	-9.52871300	3.06481000	0.59478800
H	-9.56286400	2.87775400	-1.14469000
H	-7.03161400	2.96071900	0.56391900
H	-7.06745000	2.76584300	-1.19075100
H	-8.38466900	0.86995200	0.81071200
H	-8.42164900	0.67737700	-0.91542500
H	-2.33543000	-6.42946000	-0.44956000
H	-1.49210900	-5.50459900	-1.69503300
H	-3.22159600	-5.25318000	-1.42108000
H	-1.02903000	-4.60349500	0.63207900
H	-2.74976100	-4.34142500	0.85844700
H	-1.06502600	-2.97703500	-1.30467200
H	-2.77038500	-2.73395800	-1.05124300
H	-0.55536800	-2.00609200	0.94010200
H	-2.24750000	-1.99808700	1.34712900

H	1.49211100	-5.50476500	1.69459100
H	2.33549000	-6.42949900	0.44906100
H	3.22160100	-5.25328300	1.42070500
H	1.02907300	-4.60346800	-0.63245300
H	2.74980400	-4.34135100	-0.85876000
H	1.06499300	-2.97716500	1.30442800
H	2.77035500	-2.73404600	1.05107100
H	0.55537300	-2.00603600	-0.94025500
H	2.24750900	-1.99799600	-1.34727400
Se	-4.46320186	2.26401952	-0.28632999
Se	4.43764168	2.31815512	0.29223558
Se	-0.00000800	5.27431000	0.00003000
S	-4.98305300	-1.93670600	0.17419800
S	4.98305900	-1.93669500	-0.17424700

Y6-Se-S-Se(B3)

C	9.49763200	-5.17772900	-0.63675600
C	8.14889800	-5.56437200	-0.63175700
C	7.74360700	-6.88320200	-0.74988300
C	8.73504200	-7.84067300	-0.87730500
C	10.08235900	-7.47380800	-0.88440100
C	10.48820000	-6.15300700	-0.76596000
C	9.56947500	-3.70019000	-0.49131900
C	8.20130100	-3.20614300	-0.39634300
C	7.29403100	-4.36436000	-0.48451400
C	10.75025100	-2.98161600	-0.45992800
O	6.07341300	-4.36694700	-0.44510000
C	7.82813400	-1.88147200	-0.24300000
C	6.60281000	-1.20764100	-0.13420900
F	8.41954700	-9.13772900	-0.99622300
F	11.00378400	-8.43949300	-1.01031600
C	6.54341700	0.20776800	0.02983700
C	5.18905632	0.72600588	0.11757742
C	4.26111800	-0.37754800	0.02004700
C	2.77489000	1.45340900	0.21866200
C	2.92697200	0.06954200	0.09658300
C	1.40387200	1.73627600	0.16236000
C	0.71695900	0.48883800	0.03392600
N	1.67454000	-0.52245800	-0.01217200
C	0.71191100	2.98296800	0.11250700
C	-0.71192300	2.98296900	-0.11251100
C	-1.40388300	1.73627900	-0.16240100
C	-0.71696300	0.48883700	-0.03400200
N	1.24377500	4.19262900	0.19396800

N	-1.24378700	4.19263200	-0.19394200
C	-2.77489900	1.45341000	-0.21870700
C	-2.92697800	0.06954200	-0.09662200
N	-1.67454600	-0.52245000	0.01213600
C	-5.16351514	0.78012848	-0.12354201
C	-4.26112200	-0.37755300	-0.02007900
C	-6.54342000	0.20775500	-0.02985300
C	-6.60280700	-1.20765500	0.13419400
C	-7.82812800	-1.88148800	0.24301200
C	-8.20128900	-3.20616000	0.39636700
C	-9.56946100	-3.70021100	0.49137300
C	-9.49760900	-5.17774800	0.63683000
C	-8.14887300	-5.56438500	0.63180900
C	-7.29401600	-4.36437600	0.48450900
C	-10.48817000	-6.15302800	0.76607700
C	-10.08232000	-7.47382500	0.88453800
C	-8.73500200	-7.84068400	0.87742300
C	-7.74357300	-6.88321100	0.74995900
F	-11.00373800	-8.43950900	1.01049500
F	-8.41950000	-9.13773600	0.99636200
C	-10.75024000	-2.98164000	0.46000500
O	-6.07339600	-4.36695400	0.44510900
C	12.03141300	-3.59057600	-0.56430000
N	13.08558300	-4.05915200	-0.64686400
C	10.82096900	-1.56804600	-0.32169700
N	10.91010600	-0.41955600	-0.20969200
C	13.80662500	12.25104700	1.14466200
C	12.45709900	11.53399500	1.10546700
C	12.58630100	10.01751600	0.94361400
C	11.24162700	9.28874500	0.90249100
C	11.37398400	7.77298100	0.74019000
C	10.02989600	7.04309700	0.69642200
C	10.16560600	5.52788200	0.53302300
C	8.82249300	4.79667600	0.48534700
C	8.96507100	3.28287000	0.31984300
C	7.61869000	2.55622000	0.26767400
C	7.79635200	1.04759000	0.09584100
C	-13.80667700	12.25100900	-1.14461500
C	-12.45714600	11.53396200	-1.10543700
C	-12.58634100	10.01748400	-0.94357400
C	-11.24166400	9.28871800	-0.90246700
C	-11.37401100	7.77295500	-0.74015500
C	-10.02992100	7.04307600	-0.69640400
C	-10.16562300	5.52786100	-0.53299400

C	-8.82250800	4.79665900	-0.48533900
C	-8.96508200	3.28285400	-0.31982300
C	-7.61869900	2.55620400	-0.26767800
C	-7.79635800	1.04757600	-0.09583400
C	-12.03139700	-3.59060000	0.56441200
N	-13.08557000	-4.05916300	0.64700600
C	-10.82096100	-1.56807100	0.32176300
N	-10.91011300	-0.41958300	0.20974100
C	-2.26705800	-5.44747300	-0.92411300
C	-1.95734100	-4.36016500	0.10282600
C	-1.83930500	-2.97282400	-0.53176900
C	-1.54668900	-1.89526500	0.51351900
C	2.26708100	-5.44755400	0.92369700
C	1.95736800	-4.36016700	-0.10315900
C	1.83929500	-2.97287900	0.53154800
C	1.54669000	-1.89523900	-0.51366000
H	6.69681300	-7.15947500	-0.74359700
H	11.54642900	-5.94094600	-0.77887100
H	8.65301100	-1.18757900	-0.19044200
H	-8.65300700	-1.18759900	0.19047000
H	-11.54639900	-5.94097200	0.77900800
H	-6.69677800	-7.15947900	0.74365500
H	13.68419500	13.33177500	1.26073100
H	14.37336500	12.07929300	0.22386400
H	14.41975300	11.89602800	1.97928900
H	11.85390800	11.93447900	0.28178200
H	11.90003000	11.75247100	2.02450100
H	13.14508800	9.79933500	0.02445500
H	13.19071600	9.61713700	1.76767700
H	10.63787700	9.68957800	0.07834900
H	10.68335300	9.50704500	1.82175900
H	11.93364800	7.55501700	-0.17821200
H	11.97666800	7.37198600	1.56491400
H	9.42712100	7.44378600	-0.12845700
H	9.46990200	7.25990200	1.61495200
H	10.72740700	5.31120300	-0.38414600
H	10.76662600	5.12658800	1.35856800
H	8.22111000	5.19733000	-0.34050400
H	8.26015100	5.01091300	1.40299400
H	9.52872100	3.06482200	-0.59475700
H	9.56283800	2.87777500	1.14472300
H	7.03162100	2.96073000	-0.56393500
H	7.06742500	2.76586200	1.19073600
H	8.42162700	0.67739400	0.91544700

H	8.38468400	0.86996400	-0.81069200
H	-14.41981600	11.89598300	-1.97923000
H	-14.37340000	12.07925900	-0.22380600
H	-13.68425300	13.33173700	-1.26069400
H	-11.85394400	11.93445400	-0.28176500
H	-11.90009400	11.75243500	-2.02448100
H	-13.14511100	9.79930700	-0.02440500
H	-13.19076800	9.61709800	-1.76762300
H	-10.63790100	9.68955900	-0.07833700
H	-10.68340400	9.50701500	-1.82174500
H	-11.93366100	7.55499500	0.17825800
H	-11.97670800	7.37195300	-1.56486600
H	-9.42713500	7.44377100	0.12846200
H	-9.46994200	7.25987700	-1.61494500
H	-10.72740800	5.31118600	0.38418700
H	-10.76665800	5.12656100	-1.35852600
H	-8.22111200	5.19731800	0.34050000
H	-8.26018300	5.01089200	-1.40299600
H	-9.52871300	3.06481000	0.59478800
H	-9.56286400	2.87775400	-1.14469000
H	-7.03161400	2.96071900	0.56391900
H	-7.06745000	2.76584300	-1.19075100
H	-8.38466900	0.86995200	0.81071200
H	-8.42164900	0.67737700	-0.91542500
H	-2.33543000	-6.42946000	-0.44956000
H	-1.49210900	-5.50459900	-1.69503300
H	-3.22159600	-5.25318000	-1.42108000
H	-1.02903000	-4.60349500	0.63207900
H	-2.74976100	-4.34142500	0.85844700
H	-1.06502600	-2.97703500	-1.30467200
H	-2.77038500	-2.73395800	-1.05124300
H	-0.55536800	-2.00609200	0.94010200
H	-2.24750000	-1.99808700	1.34712900
H	1.49211100	-5.50476500	1.69459100
H	2.33549000	-6.42949900	0.44906100
H	3.22160100	-5.25328300	1.42070500
H	1.02907300	-4.60346800	-0.63245300
H	2.74980400	-4.34135100	-0.85876000
H	1.06499300	-2.97716500	1.30442800
H	2.77035500	-2.73404600	1.05107100
H	0.55537300	-2.00603600	-0.94025500
H	2.24750900	-1.99799600	-1.34727400
Se	-0.00000800	5.27431000	0.00003000
S	-4.46320186	2.26401952	-0.28632999

S	4.43764168	2.31815512	0.29223558
Se	-4.98305300	-1.93670600	0.17419800
Se	4.98305900	-1.93669500	-0.17424700

Y6-Se-Se-Se(B4)

C	9.49763200	-5.17772900	-0.63675600
C	8.14889800	-5.56437200	-0.63175700
C	7.74360700	-6.88320200	-0.74988300
C	8.73504200	-7.84067300	-0.87730500
C	10.08235900	-7.47380800	-0.88440100
C	10.48820000	-6.15300700	-0.76596000
C	9.56947500	-3.70019000	-0.49131900
C	8.20130100	-3.20614300	-0.39634300
C	7.29403100	-4.36436000	-0.48451400
C	10.75025100	-2.98161600	-0.45992800
O	6.07341300	-4.36694700	-0.44510000
C	7.82813400	-1.88147200	-0.24300000
C	6.60281000	-1.20764100	-0.13420900
F	8.41954700	-9.13772900	-0.99622300
F	11.00378400	-8.43949300	-1.01031600
C	6.54341700	0.20776800	0.02983700
C	5.18905632	0.72600588	0.11757742
C	4.26111800	-0.37754800	0.02004700
C	2.77489000	1.45340900	0.21866200
C	2.92697200	0.06954200	0.09658300
C	1.40387200	1.73627600	0.16236000
C	0.71695900	0.48883800	0.03392600
N	1.67454000	-0.52245800	-0.01217200
C	0.71191100	2.98296800	0.11250700
C	-0.71192300	2.98296900	-0.11251100
C	-1.40388300	1.73627900	-0.16240100
C	-0.71696300	0.48883700	-0.03400200
N	1.24377500	4.19262900	0.19396800
N	-1.24378700	4.19263200	-0.19394200
C	-2.77489900	1.45341000	-0.21870700
C	-2.92697800	0.06954200	-0.09662200
N	-1.67454600	-0.52245000	0.01213600
C	-5.16351514	0.78012848	-0.12354201
C	-4.26112200	-0.37755300	-0.02007900
C	-6.54342000	0.20775500	-0.02985300
C	-6.60280700	-1.20765500	0.13419400
C	-7.82812800	-1.88148800	0.24301200
C	-8.20128900	-3.20616000	0.39636700
C	-9.56946100	-3.70021100	0.49137300

C	-9.49760900	-5.17774800	0.63683000
C	-8.14887300	-5.56438500	0.63180900
C	-7.29401600	-4.36437600	0.48450900
C	-10.48817000	-6.15302800	0.76607700
C	-10.08232000	-7.47382500	0.88453800
C	-8.73500200	-7.84068400	0.87742300
C	-7.74357300	-6.88321100	0.74995900
F	-11.00373800	-8.43950900	1.01049500
F	-8.41950000	-9.13773600	0.99636200
C	-10.75024000	-2.98164000	0.46000500
O	-6.07339600	-4.36695400	0.44510900
C	12.03141300	-3.59057600	-0.56430000
N	13.08558300	-4.05915200	-0.64686400
C	10.82096900	-1.56804600	-0.32169700
N	10.91010600	-0.41955600	-0.20969200
C	13.80662500	12.25104700	1.14466200
C	12.45709900	11.53399500	1.10546700
C	12.58630100	10.01751600	0.94361400
C	11.24162700	9.28874500	0.90249100
C	11.37398400	7.77298100	0.74019000
C	10.02989600	7.04309700	0.69642200
C	10.16560600	5.52788200	0.53302300
C	8.82249300	4.79667600	0.48534700
C	8.96507100	3.28287000	0.31984300
C	7.61869000	2.55622000	0.26767400
C	7.79635200	1.04759000	0.09584100
C	-13.80667700	12.25100900	-1.14461500
C	-12.45714600	11.53396200	-1.10543700
C	-12.58634100	10.01748400	-0.94357400
C	-11.24166400	9.28871800	-0.90246700
C	-11.37401100	7.77295500	-0.74015500
C	-10.02992100	7.04307600	-0.69640400
C	-10.16562300	5.52786100	-0.53299400
C	-8.82250800	4.79665900	-0.48533900
C	-8.96508200	3.28285400	-0.31982300
C	-7.61869900	2.55620400	-0.26767800
C	-7.79635800	1.04757600	-0.09583400
C	-12.03139700	-3.59060000	0.56441200
N	-13.08557000	-4.05916300	0.64700600
C	-10.82096100	-1.56807100	0.32176300
N	-10.91011300	-0.41958300	0.20974100
C	-2.26705800	-5.44747300	-0.92411300
C	-1.95734100	-4.36016500	0.10282600
C	-1.83930500	-2.97282400	-0.53176900

C	-1.54668900	-1.89526500	0.51351900
C	2.26708100	-5.44755400	0.92369700
C	1.95736800	-4.36016700	-0.10315900
C	1.83929500	-2.97287900	0.53154800
C	1.54669000	-1.89523900	-0.51366000
H	6.69681300	-7.15947500	-0.74359700
H	11.54642900	-5.94094600	-0.77887100
H	8.65301100	-1.18757900	-0.19044200
H	-8.65300700	-1.18759900	0.19047000
H	-11.54639900	-5.94097200	0.77900800
H	-6.69677800	-7.15947900	0.74365500
H	13.68419500	13.33177500	1.26073100
H	14.37336500	12.07929300	0.22386400
H	14.41975300	11.89602800	1.97928900
H	11.85390800	11.93447900	0.28178200
H	11.90003000	11.75247100	2.02450100
H	13.14508800	9.79933500	0.02445500
H	13.19071600	9.61713700	1.76767700
H	10.63787700	9.68957800	0.07834900
H	10.68335300	9.50704500	1.82175900
H	11.93364800	7.55501700	-0.17821200
H	11.97666800	7.37198600	1.56491400
H	9.42712100	7.44378600	-0.12845700
H	9.46990200	7.25990200	1.61495200
H	10.72740700	5.31120300	-0.38414600
H	10.76662600	5.12658800	1.35856800
H	8.22111000	5.19733000	-0.34050400
H	8.26015100	5.01091300	1.40299400
H	9.52872100	3.06482200	-0.59475700
H	9.56283800	2.87777500	1.14472300
H	7.03162100	2.96073000	-0.56393500
H	7.06742500	2.76586200	1.19073600
H	8.42162700	0.67739400	0.91544700
H	8.38468400	0.86996400	-0.81069200
H	-14.41981600	11.89598300	-1.97923000
H	-14.37340000	12.07925900	-0.22380600
H	-13.68425300	13.33173700	-1.26069400
H	-11.85394400	11.93445400	-0.28176500
H	-11.90009400	11.75243500	-2.02448100
H	-13.14511100	9.79930700	-0.02440500
H	-13.19076800	9.61709800	-1.76762300
H	-10.63790100	9.68955900	-0.07833700
H	-10.68340400	9.50701500	-1.82174500
H	-11.93366100	7.55499500	0.17825800

H	-11.97670800	7.37195300	-1.56486600
H	-9.42713500	7.44377100	0.12846200
H	-9.46994200	7.25987700	-1.61494500
H	-10.72740800	5.31118600	0.38418700
H	-10.76665800	5.12656100	-1.35852600
H	-8.22111200	5.19731800	0.34050000
H	-8.26018300	5.01089200	-1.40299600
H	-9.52871300	3.06481000	0.59478800
H	-9.56286400	2.87775400	-1.14469000
H	-7.03161400	2.96071900	0.56391900
H	-7.06745000	2.76584300	-1.19075100
H	-8.38466900	0.86995200	0.81071200
H	-8.42164900	0.67737700	-0.91542500
H	-2.33543000	-6.42946000	-0.44956000
H	-1.49210900	-5.50459900	-1.69503300
H	-3.22159600	-5.25318000	-1.42108000
H	-1.02903000	-4.60349500	0.63207900
H	-2.74976100	-4.34142500	0.85844700
H	-1.06502600	-2.97703500	-1.30467200
H	-2.77038500	-2.73395800	-1.05124300
H	-0.55536800	-2.00609200	0.94010200
H	-2.24750000	-1.99808700	1.34712900
H	1.49211100	-5.50476500	1.69459100
H	2.33549000	-6.42949900	0.44906100
H	3.22160100	-5.25328300	1.42070500
H	1.02907300	-4.60346800	-0.63245300
H	2.74980400	-4.34135100	-0.85876000
H	1.06499300	-2.97716500	1.30442800
H	2.77035500	-2.73404600	1.05107100
H	0.55537300	-2.00603600	-0.94025500
H	2.24750900	-1.99799600	-1.34727400
Se	-4.46320186	2.26401952	-0.28632999
Se	4.43764168	2.31815512	0.29223558
Se	-4.98305300	-1.93670600	0.17419800
Se	4.98305900	-1.93669500	-0.17424700
Se	-0.00000800	5.27431000	0.00003000