

Electronic Supplementary Information for

Narrowband TADF emitters with high utilization of triplet excitons: theoretical insight and molecular design

Qing Zhang,^a Tao Liu,^a Zhouyang Shi,^b Zhong Zheng,^c Chunyan Lv,^{*a} Xin Wang,^{*d}
Yujian Zhang^{*c}

^[a]Department of Materials Chemistry, Huzhou University, East 2nd Ring Rd. No. 759, Huzhou, 313000, People's Republic of China, E-mail: lcy@zjhu.edu.cn

^[b]Zhejiang Jiuhe Geological and Ecological Environment Planning and Design Co., LTD, Huzhou, 313002, People's Republic of China

^[c]Anji Branch of Huzhou Ecological Environment Bureau, Huzhou, 313300, People's Republic of China

^[d]Henan-Macquarie University Joint Centre for Biomedical Innovation, Henan Key Laboratory of Brain Targeted Bio-nanomedicine, School of Life Sciences, Henan University, Kaifeng, Henan, 475004, People's Republic of China, E-mail: wx@henu.edu.cn

^[e]Key Laboratory of the Ministry of Education for Advanced Catalysis Materials, Department of Chemistry, Zhejiang Normal University, Yingbin Road No. 688, Jinhua 321004, People's Republic of China, sciencezyj@foxmail.com

1. Definition of MPP and SDP

The molecular planarity parameter (MPP) and span of deviation from plane (SDP) are two reliable metrics to evaluate the planarity of the whole molecule. For a given molecule with N atoms, the MPP can be defined as the root-mean-square of deviation of atoms from the fitting plane

$$MPP = \sqrt{\frac{1}{N} \sum_i d_i^2}$$

where d_i is the distance between the atom i and the fitting plane. The signed distance between the atom i and the fitting plane can be evaluated as

$$d_i^s = \frac{Ax_i + By_i + Cz_i + D}{\sqrt{A^2 + B^2 + C^2}}$$

where A, B, C, D are parameters of the fitting plane. Following that, the SDP can be simply calculated as

$$SDP = d_{\max}^s - d_{\min}^s$$

in which the d_{\max}^s and d_{\min}^s are the most positive and the most negative d^s values among all the considered atoms, respectively.

2. Definition of D -index and S_r -index

The charge transfer length in the X/Y/Z direction can be calculated by evaluating the distance between centroid of hole and electron in the corresponding directions:

$$D_x = |X_{\text{ele}} - X_{\text{hole}}|, D_y = |Y_{\text{ele}} - Y_{\text{hole}}|, D_z = |Z_{\text{ele}} - Z_{\text{hole}}|$$

Based on the abovementioned definitions, the total magnitude of the charge transfer length can be defined as D -index:

$$D\text{-index} = \sqrt{(D_x)^2 + (D_y)^2 + (D_z)^2}$$

The overlap function between the hole and electron distribution can be defined as

$$S_r(r) = \sqrt{\rho^{\text{hole}}(r)\rho^{\text{ele}}(r)}$$

where ρ^{hole} and ρ^{ele} are the density distribution of hole and electron, respectively. The S_r -index refers to the overlapping extent of the hole and electron, and it can be defined as the integral of the S_r function:

$$S_r - \text{index} = \int S_r(r) dr = \sqrt{\rho^{\text{hole}}(r)\rho^{\text{ele}}(r)}$$

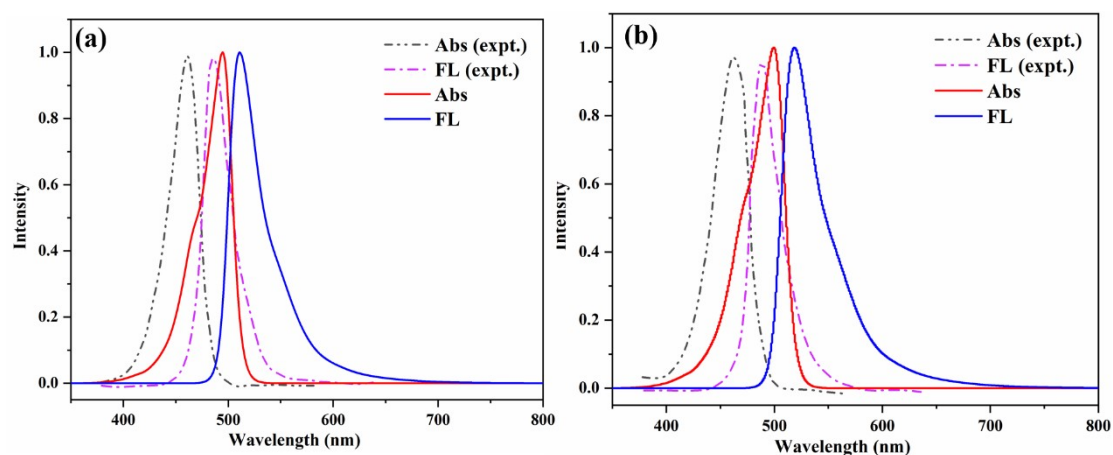


Fig. S1 B3LYP-simulated absorption (Abs) and the normalized vibrational resolved fluorescence spectrum (FL) of **BN-DMAC** and **BN-DPAC**, together with their corresponding curves measured in the experiment.¹⁶

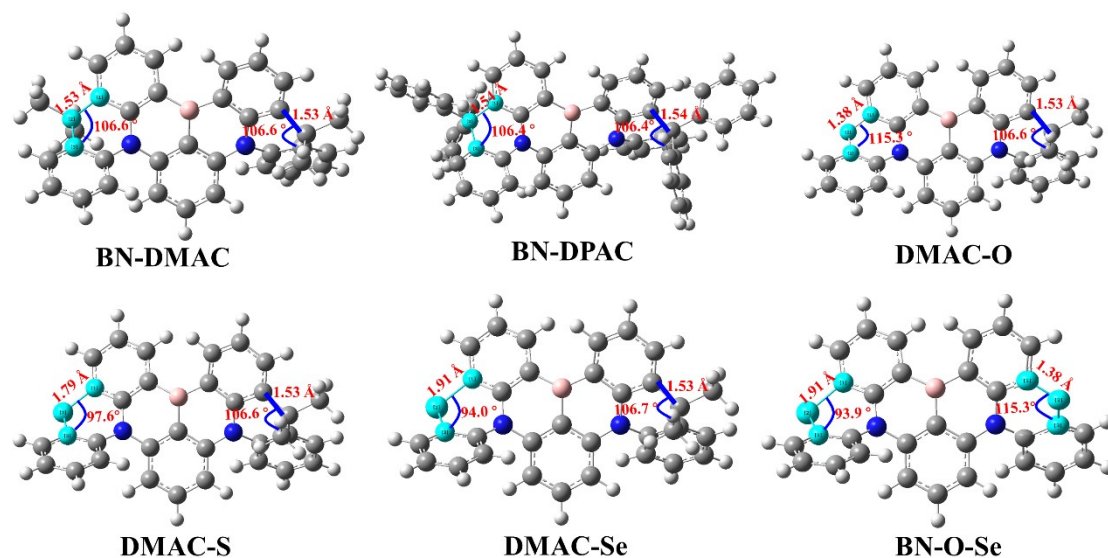


Fig. S2 B3LYP-optimized structures for all studied MR-TADF emitters, together with the bond lengths and angle degrees between the sp^3 -inserted C and its neighboring C atoms.

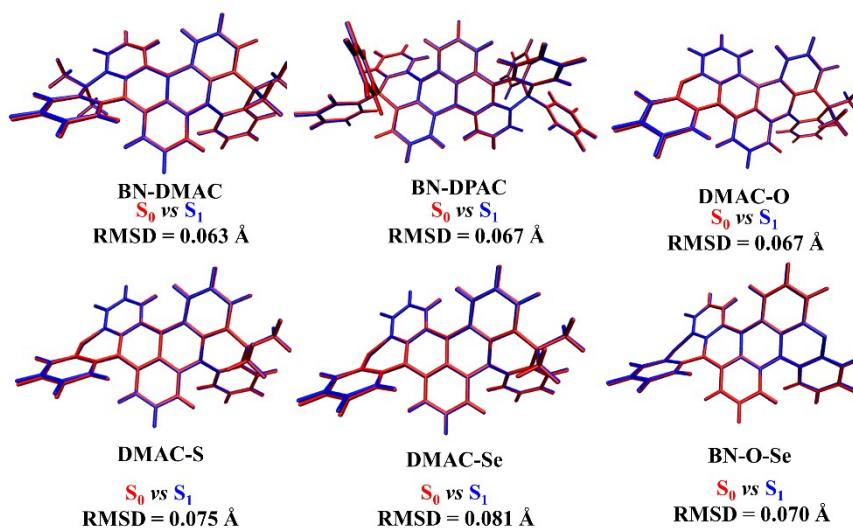


Fig. S3. Geometry comparison and RMSD values for the S_0 (red) vs S_1 (blue) of all the considered systems here.

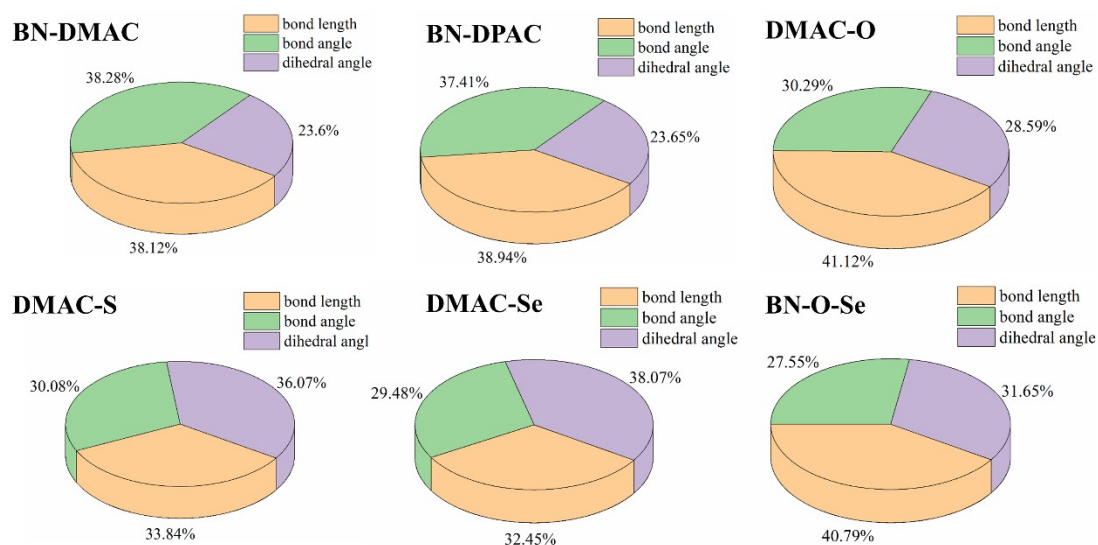


Fig. S4. Contributions of bond lengths, bond angles, and dihedral angles to the reorganization energy between S_0 and S_1 at S_1 -optimized geometries for all studied systems.

Table S1. Emission energies of S_1 and T_1 , the maximum wavelength of fluorescence (λ_{emi}), and S_1 - T_1 energy gaps (ΔE_{ST}) simulated by combining B3LYP, BMK, and PBE0 functionals with 6-31G(d, p) basis sets, respectively, as well as the λ and ΔE_{ST} values measured in the experiment.¹⁶

		S_1 (eV)	λ_{emi} (nm)	T_1 (eV)	ΔE_{ST} (eV)
BN-DMAC	B3LYP	2.62	474	2.28	0.33
	BMK	2.94	421	2.51	0.43
	PBE0	2.73	455	2.35	0.38
	Expt.	2.56	485	-	0.14
BN-DPAC	B3LYP	2.59	480	2.27	0.32
	BMK	2.91	425	2.50	0.41
	PBE0	2.69	461	2.33	0.36
	Expt.	2.53	490	-	0.11

Table S2. B3LYP-predicted vertical excitation energies (ΔE_{emi} , eV), maximum wavelengths of the fluorescence (λ_{emi} , nm), transition dipole moments (μ , Debye) and oscillator strengths (f) for the $S_1 \rightarrow S_0$ transitions of all systems considered here.

	BN-DMAC	BN-DPAC	DMAC-O	DMAC-S	DMAC-Se	BN-O-Se
ΔE_{emi}	2.62	2.59	2.52	2.53	2.53	2.46
λ_{emi}	474	480	492	490	489	504
f	0.328	0.349	0.275	0.275	0.268	0.245
μ	5.75	5.97	5.37	5.35	5.28	5.13
λ_{expt}	485	490				

Table S3. Calculated vertical excitation energies of S_1 (ΔE_{S1} , eV) and T_1 (ΔE_{T1} , eV), fluorescence peaks (λ_{emi} , nm), and energy gaps between S_1 and T_1 (ΔE_{ST} , eV) by the wavefunction-based STEOM-DLPNO-CCSD/def2-SVP calculations, together with the fluorescence peaks (λ_{expt} , nm) and energy gaps between S_1 and T_1 (ΔE_{expt} , eV) measured in the experiment.¹⁶

	BN-DMAC	BN-DPAC	DMAC-O	DMAC-S	DMAC-Se	BN-O-Se
S_1 (eV)	2.571	2.544	2.543	2.527	2.561	2.503
λ_{emi} (nm)	483	488	488	491	484	496
T_1 (eV)	2.448	2.425	2.376	2.395	2.407	2.343
ΔE_{ST}	0.123	0.119	0.167	0.132	0.154	0.160
λ_{expt}	485	490				
ΔE_{expt}	0.14	0.11				

Table S4. Total reorganization energy and the corresponding contributions of bond lengths, bond angles, and dihedral angles of all the studied molecules, where the energy is in meV.

	Bond length	Bond angle	Dihedral angle	Total
BN-DMAC	38.2	38.3	23.6	100.1
BN-DPAC	39.8	38.2	24.2	102.2
DMAC-O	48.7	35.8	33.8	118.4
DMAC-S	40.8	36.3	43.5	120.6
DMAC-Se	40.0	36.3	47.0	123.4
BN-O-Se	53.3	36.0	41.4	130.7

Table S5: Cartesian coordinates of the (TD) B3LYP-optimized S_0 , S_1 , and T_1 structures for all the studied MR-TADF emitters.

				MR-TADF			
				emitters.			
<hr/>				H	6.78120500	-2.13968400	-2.60899400
BN	DMAC_ S_0			C	3.85727300	2.68890900	1.20594100
N	2.43340400	-0.46220800	-0.06385900	H	4.80932000	3.08286600	1.54290700
N	-2.43339300	-0.46234900	0.06357700	C	-4.91182400	0.34838700	-0.96281200
C	-1.22250100	-1.18217300	0.03914900	C	4.66148600	-0.52090600	2.23094300
C	1.21913000	-2.58465700	-0.02022400	H	4.65723200	0.11041200	3.12541100
H	2.14767100	-3.14171600	-0.01374600	H	5.45488200	-1.26826900	2.33638100
C	-1.50623800	3.03574300	-0.82023400	H	3.70416300	-1.04447100	2.17921200
H	-0.63256400	3.67708100	-0.87267200	C	4.91161800	0.34844100	0.96316900
C	3.76009000	1.35274700	0.82344400	C	5.99194000	-0.98341400	-0.97337300
C	3.59488300	-0.96876000	-0.72515500	H	6.97626800	-0.67043800	-0.64515400
C	0.00001200	-0.46337600	-0.00014300	C	-5.88527200	-1.81232000	2.09031800
C	1.34784600	1.70434800	0.38125700	H	-6.78057800	-2.13991800	2.60967600
C	-3.59469300	-0.96897500	0.72508400	C	-4.62392800	-2.20280700	2.53876600
C	3.48276900	-1.77155100	-1.86928200	H	-4.52167000	-2.82668000	3.42161700
H	2.50258300	-2.04744400	-2.23880500	C	-4.66202100	-0.52088300	-2.23073000
C	-2.50217800	0.87816000	-0.38263600	H	-4.65795000	0.11051500	-3.12514100
C	2.50209000	0.87828200	0.38245200	H	-5.45548600	-1.26818700	-2.33602800
C	-3.76027800	1.35264300	-0.82332900	H	-3.70471400	-1.04450300	-2.17927500
C	1.22260000	-1.18209800	-0.03956000	C	6.27539100	1.03891400	1.12569600
C	4.86035200	-0.55163700	-0.27261500	H	6.51840200	1.67546400	0.26953900
C	2.74036800	3.53328300	1.20709900	H	7.07050700	0.29772700	1.24142500
H	2.84322200	4.56354300	1.53441900	H	6.29058800	1.65425400	2.02888500
C	-3.48232300	-1.77193700	1.86905400	C	-6.27555200	1.03903600	-1.12500300
H	-2.50206000	-2.04796000	2.23827300	H	-6.51840000	1.67543100	-0.26867900
C	-4.86029200	-0.55176600	0.27290900	H	-7.07075700	0.29795300	-1.24079700
C	0.00006800	-3.25878100	-0.00041700	H	-6.29077500	1.65459000	-2.02804800
H	0.00012100	-4.34513200	-0.00053600	B	-0.00005100	1.05563600	-0.00014900
C	-1.34796200	1.70427000	-0.38157800	BN-DMAC_ S_1			
C	1.50601300	3.03582700	0.81993100	N	2.41582600	-0.42755400	-0.10012000
H	0.63231400	3.67714400	0.87220600	N	-2.41582600	-0.42755400	0.10011900
C	-3.85757500	2.68880100	-1.20577600	C	-1.20267900	-1.13883100	0.06147900
H	-4.80971500	3.08273100	-1.54252400	C	1.20952800	-2.55432800	-0.01175800
C	-5.99169800	-0.98352200	0.97395100	H	2.14691300	-3.09610100	0.02279900
H	-6.97610600	-0.67043200	0.64607100	C	-1.55922200	3.08981400	-0.78618900
C	4.62452700	-2.20240300	-2.53873600	H	-0.71056900	3.76538900	-0.81175100
H	4.52249700	-2.82614800	-3.42170000	C	3.76958800	1.34857200	0.83816900
C	-2.74067800	3.53318200	-1.20717600	C	3.55412000	-0.95604300	-0.74702500
H	-2.84361400	4.56344200	-1.53447400	C	0.00000000	-0.41241300	0.00000000
C	-1.21902200	-2.58472200	0.01952500	C	1.35263300	1.75239400	0.37100700
H	-2.14757200	-3.14176900	0.01295700	C	-3.55411900	-0.95604300	0.74702500
C	5.88577400	-1.81206500	-2.08986000	C	3.42158000	-1.77714100	-1.88331500

H	2.43385900	-2.01001700	-2.26287500	H	-5.45268000	-1.31310100	-2.30124100
C	-2.51064700	0.91513700	-0.39499000	H	-3.70173500	-1.06651600	-2.16734400
C	2.51064700	0.91513800	0.39498900	C	6.28504500	0.99402700	1.09754900
C	-3.76958900	1.34857200	-0.83816800	H	6.52607100	1.63201500	0.24212000
C	1.20267900	-1.13883100	-0.06148100	H	7.07103900	0.24121500	1.20112100
C	4.83330800	-0.56356900	-0.29264100	H	6.31747100	1.60461800	2.00301300
C	2.80736400	3.55292000	1.18685200	C	-6.28504600	0.99402800	-1.09754400
H	2.92942100	4.58957300	1.49013100	H	-6.52607100	1.63201600	-0.24211500
C	-3.42157900	-1.77714300	1.88331400	H	-7.07104000	0.24121700	-1.20111500
H	-2.43385700	-2.01001900	2.26287300	H	-6.31747400	1.60462000	-2.00300800
C	-4.83330800	-0.56356900	0.29264300	B	0.00000000	1.12110300	0.00000000
C	0.00000000	-3.24850600	-0.00000400				
H	0.00000000	-4.33311800	-0.00000500	BN-DMAC_T1			
C	-1.35263400	1.75239400	-0.37100800	N	2.42188200	-0.42480300	-0.09944000
C	1.55922200	3.08981500	0.78618700	N	-2.42188200	-0.42480300	0.09943600
H	0.71057000	3.76539000	0.81174900	C	-1.20569300	-1.13658700	0.05468100
C	-3.90752700	2.69254500	-1.22300700	C	1.20938200	-2.54636800	-0.00344600
H	-4.86651100	3.06926500	-1.55616600	H	2.14706400	-3.08840500	0.03080100
C	-5.94939000	-1.04052200	0.98406000	C	-1.56421700	3.09198300	-0.76792000
H	-6.94280200	-0.75563000	0.65814000	H	-0.71559900	3.76734500	-0.79599100
C	4.55121200	-2.24804000	-2.54134000	C	3.77872600	1.35444100	0.82280800
H	4.43743600	-2.87500200	-3.42023600	C	3.56395700	-0.96166300	-0.74220700
C	-2.80736400	3.55292000	-1.18685300	C	0.00000000	-0.39996000	-0.00000300
H	-2.92942000	4.58957200	-1.49013300	C	1.35603900	1.75298700	0.35920100
C	-1.20952800	-2.55432800	0.01175200	C	-3.56395200	-0.96166500	0.74220700
H	-2.14691300	-3.09610000	-0.02280700	C	3.43055200	-1.78334400	-1.87581700
C	5.82111700	-1.88315500	-2.09058700	H	2.44283800	-2.01623000	-2.25499900
H	6.70894100	-2.23837800	-2.60440400	C	-2.51649500	0.91574900	-0.38222700
C	3.90752700	2.69254500	1.22300700	C	2.51649400	0.91575000	0.38222200
H	4.86651100	3.06926500	1.55616700	C	-3.77872900	1.35444200	-0.82280700
C	-4.90797200	0.32580200	-0.94814000	C	1.20569500	-1.13658700	-0.05469000
C	4.66664600	-0.55568600	2.21104000	C	4.84124100	-0.57222700	-0.28538600
H	4.67914400	0.06874500	3.10985500	C	2.81148100	3.55666300	1.16130200
H	5.45267600	-1.31310200	2.30124300	H	2.93392200	4.59426600	1.46110000
H	3.70173200	-1.06651500	2.16734600	C	-3.43054200	-1.78335100	1.87581300
C	4.90797000	0.32580100	0.94814200	H	-2.44282700	-2.01624000	2.25498900
C	5.94939100	-1.04052200	-0.98405700	C	-4.84123900	-0.57222600	0.28539500
H	6.94280300	-0.75563000	-0.65813600	C	0.00000000	-3.24601700	-0.00001400
C	-5.82111500	-1.88315700	2.09058800	H	0.00000000	-4.33008100	-0.00001900
H	-6.70893900	-2.23838000	2.60440600	C	-1.35603900	1.75298600	-0.35920900
C	-4.55121000	-2.24804200	2.54134000	C	1.56421700	3.09198600	0.76791000
H	-4.43743300	-2.87500600	3.42023500	H	0.71559900	3.76734800	0.79597800
C	-4.66664900	-0.55568600	-2.21103800	C	-3.91548900	2.69609800	-1.19872400
H	-4.67914700	0.06874600	-3.10985300	H	-4.87317300	3.07617000	-1.53172900
				C	-5.95879800	-1.05690700	0.97001800

H	-6.95203600	-0.77463100	0.64140500	C	8.76157200	2.42913000	-0.67467400
C	4.56084500	-2.26022100	-2.52969400	H	9.68682900	2.96932900	-0.85241500
H	4.44713000	-2.88918400	-3.40711800	C	8.62817600	1.60621200	0.44055200
C	-2.81148200	3.55666100	-1.16130800	H	9.45079600	1.49920100	1.14184900
H	-2.93392300	4.59426400	-1.46110600	C	7.43588300	0.91028500	0.67005100
C	-1.20938200	-2.54636800	0.00342500	H	7.35546500	0.27641700	1.54491100
H	-2.14706500	-3.08840300	-0.03082600	C	5.01783600	0.27589600	-0.00209300
C	5.83054100	-1.90151400	-2.07450600	C	5.05412400	-0.58503300	1.29709300
H	6.71856300	-2.26305000	-2.58355600	C	5.53381600	-1.90263700	1.27129800
C	3.91548600	2.69609800	1.19872500	H	5.84405100	-2.34379400	0.33045800
H	4.87316900	3.07616800	1.53173500	C	5.61743800	-2.66208400	2.43944900
C	-4.91457700	0.32998600	-0.94633700	H	5.99011500	-3.68133800	2.38942700
C	4.66655100	-0.53698400	2.21758500	C	5.22165100	-2.11939700	3.66222600
H	4.67892000	0.09657600	3.10997900	H	5.28104300	-2.71094800	4.57112900
H	5.45010900	-1.29559300	2.31740100	C	4.74652100	-0.80845000	3.70284600
H	3.70040000	-1.04563000	2.17692500	H	4.43288900	-0.37056600	4.64625800
C	4.91457200	0.32998400	0.94634800	C	4.66475400	-0.05062600	2.53331400
C	5.95880300	-1.05690600	-0.97000500	H	4.28901200	0.96492000	2.58702300
H	6.95204000	-0.77463200	-0.64138700	C	4.71668100	-0.63895100	-1.20108800
C	-5.83053100	-1.90152000	2.07451400	C	5.69754600	-1.10603800	-2.08395500
H	-6.71855000	-2.26305800	2.58356700	H	6.72719700	-0.80260600	-1.93467900
C	-4.56083300	-2.26023000	2.52969400	C	5.37768900	-1.95100100	-3.14530100
H	-4.44711400	-2.88919800	3.40711400	H	6.15929000	-2.30668800	-3.80934200
C	-4.66656900	-0.53698300	-2.21757700	C	4.04860800	-2.32128900	-3.35145900
H	-4.67895700	0.09657500	-3.10997200	H	3.77635000	-2.95287000	-4.19172500
H	-5.45012200	-1.29559900	-2.31737900	C	3.05656700	-1.86521200	-2.48911300
H	-3.70041200	-1.04562000	-2.17693100	H	2.02182500	-2.13265200	-2.66510300
C	6.29238300	0.99706700	1.09285100	C	3.38702400	-1.05209000	-1.39450800
H	6.53674000	1.62628100	0.23191500	C	2.52965700	0.79228100	-0.10207300
H	7.07652400	0.24370200	1.20541400	C	3.84517800	1.27358400	0.08812200
H	6.32407300	1.61608100	1.99259400	C	4.01062900	2.60088300	0.48065100
C	-6.29239000	0.99706900	-1.09282700	H	5.01232500	2.98092000	0.64541300
H	-6.53672800	1.62630300	-0.23189900	C	1.62894500	2.94226000	0.54233200
H	-7.07653500	0.24370200	-1.20535500	H	0.77809000	3.57908200	0.76193700
H	-6.32409900	1.61606100	-1.99258300	C	2.91293000	3.43866300	0.70778600
B	0.00000000	1.11760200	-0.00000400	H	3.07356800	4.46155300	1.03453900
BN-DPAC_S₀				C	1.39501100	1.61654300	0.12301300
N	-2.37711900	-0.54602400	0.52422200	C	-0.00001700	-0.54950300	-0.00003300
N	2.37707500	-0.54597300	-0.52430200	C	1.19345100	-1.26744300	-0.26671200
C	6.35532500	1.02406400	-0.21081300	C	1.19508800	-2.66907700	-0.24242600
C	6.50493400	1.85927500	-1.33312000	H	2.11053700	-3.22525200	-0.40005400
H	5.68013300	1.96531900	-2.03096600	C	-0.00000200	-3.34305300	-0.00003300
C	7.68985900	2.55291100	-1.56391900	H	0.00000400	-4.42934200	-0.00003700
H	7.77685700	3.19092000	-2.43876900	C	-1.19348900	-1.26745500	0.26661100

C	-1.19510100	-2.66909400	0.24232900	B	-0.00001800	0.96809500	0.00002000
H	-2.11054300	-3.22527100	0.39999800	BN-DPAC_S₁			
C	-2.52969200	0.79228200	0.10216200	N	-2.35210200	0.48867100	-0.55238200
C	-1.39505700	1.61656300	-0.12284500	N	2.35211000	0.48864000	0.55244100
C	-1.62898800	2.94235900	-0.54194700	C	6.35926600	-0.99316700	0.21325700
H	-0.77811900	3.57919600	-0.76147300	C	6.51069700	-1.83366600	1.33119900
C	-2.91297500	3.43878000	-0.70730500	H	5.67778300	-1.96387700	2.01515200
H	-3.07364100	4.46170900	-1.03391500	C	7.70729200	-2.50317700	1.57307600
C	-4.01067300	2.60095900	-0.48028900	H	7.79603500	-3.14679900	2.44363700
H	-5.01236800	2.98102400	-0.64498800	C	8.78762100	-2.35014100	0.69890200
C	-3.84521400	1.27361000	-0.08794200	H	9.72164300	-2.87220300	0.88498400
C	-4.71672000	-0.63906300	1.20101600	C	8.65149600	-1.52276600	-0.41278100
C	-3.38708100	-1.05226000	1.39436900	H	9.48064200	-1.39400200	-1.10266600
C	-3.05663200	-1.86560300	2.48880500	C	7.44774000	-0.85037400	-0.65307700
H	-2.02189900	-2.13311800	2.66473100	H	7.36469300	-0.21287300	-1.52512900
C	-4.04868600	-2.32184900	3.35105900	C	5.00929400	-0.27083100	-0.00478000
H	-3.77642600	-2.95360000	4.19119400	C	5.04218600	0.60233600	-1.29686800
C	-5.37775900	-1.95150600	3.14496600	C	5.50395200	1.92624700	-1.26396600
H	-6.15938500	-2.30735300	3.80889500	H	5.81085600	2.36725600	-0.32187200
C	-5.69760000	-1.10633500	2.08376800	C	5.57591900	2.69345800	-2.42836200
H	-6.72725400	-0.80290200	1.93452800	H	5.93463900	3.71750700	-2.37313700
C	-5.01786200	0.27591000	0.00212700	C	5.18750400	2.15156600	-3.65359200
C	-6.35534400	1.02410100	0.21086100	H	5.23905400	2.74836100	-4.55957600
C	-6.50501900	1.85909700	1.33330400	C	4.73030100	0.83404400	-3.70092600
H	-5.68027800	1.96497600	2.03125100	H	4.42341100	0.39659400	-4.64674400
C	-7.68992400	2.55276800	1.56408700	C	4.65794900	0.06914000	-2.53567300
H	-7.77696600	3.19063400	2.43903700	H	4.29595700	-0.95124600	-2.59157700
C	-8.76153200	2.42925500	0.67468000	C	4.68895100	0.63038200	1.19788600
H	-9.68677400	2.96947500	0.85242300	C	5.65955100	1.13736700	2.06620500
C	-8.62807300	1.60652700	-0.44067500	H	6.69592200	0.85795600	1.91674500
H	-9.45063600	1.49966000	-1.14206300	C	5.32507200	1.99473800	3.11602800
C	-7.43578500	0.91057400	-0.67016400	H	6.10267300	2.37404400	3.77148400
H	-7.35527700	0.27689700	-1.54515700	C	3.98924900	2.34281700	3.32789600
C	-5.05407300	-0.58494200	-1.29710600	H	3.71071500	2.97706600	4.16369900
C	-4.66486300	-0.05047100	-2.53334100	C	3.00311800	1.84950300	2.48301800
H	-4.28927800	0.96513000	-2.58708400	H	1.96055400	2.07416700	2.67367700
C	-4.74660100	-0.80829400	-3.70288900	C	3.34739600	1.01959900	1.39780500
H	-4.43308000	-0.37034500	-4.64630700	C	2.53923700	-0.85184900	0.08689300
C	-5.22151800	-2.11930700	-3.66225100	C	3.85616800	-1.28909900	-0.11395800
H	-5.28082300	-2.71089700	-4.57113500	C	4.06246300	-2.62323400	-0.50459700
C	-5.61710800	-2.66207700	-2.43943300	H	5.06948200	-2.98272800	-0.67443000
H	-5.98958900	-3.68140200	-2.38939500	C	1.67476900	-3.02124200	-0.50288900
C	-5.53351400	-1.90264400	-1.27128800	H	0.84372000	-3.69336000	-0.69013800
H	-5.84357300	-2.34387000	-0.33042100	C	2.97391300	-3.48022700	-0.68581400

H	3.14909100	-4.50919100	-0.98874300	H	-4.29615600	-0.95163700	2.59154000
C	1.39708000	-1.68832200	-0.11495400	C	-4.73039400	0.83357200	3.70106000
C	0.00000400	0.47496200	0.00002800	H	-4.42360000	0.39598900	4.64684700
C	1.17000300	1.19991400	0.28372000	C	-5.18747100	2.15114200	3.65384500
C	1.18714800	2.61586600	0.23233600	H	-5.23901700	2.74784200	4.55989200
H	2.11674900	3.15626700	0.36157000	C	-5.57576500	2.69320500	2.42865200
C	-0.00001000	3.30916200	0.00017100	H	-5.93438700	3.71729400	2.37352000
H	-0.00001600	4.39373600	0.00022600	C	-5.50380300	1.92611600	1.26417600
C	-1.17000100	1.19993100	-0.28359000	H	-5.81060900	2.36725800	0.32211300
C	-1.18716100	2.61587700	-0.23206400	B	0.00001100	-1.05832800	-0.00004800
H	-2.11676800	3.15628100	-0.36124200	BN-DPAC_T1			
C	-2.53921900	-0.85186700	-0.08696600	N	-2.35878200	0.49211800	-0.55050100
C	-1.39705100	-1.68834600	0.11480700	N	2.35877300	0.49215000	0.55043100
C	-1.67472300	-3.02129900	0.50263800	C	6.36591700	-0.99073400	0.21748800
H	-0.84366600	-3.69342200	0.68983000	C	6.52253500	-1.81608300	1.34592000
C	-2.97386000	-3.48030800	0.68554600	H	5.69350600	-1.93600000	2.03643700
H	-3.14902500	-4.50929400	0.98840700	C	7.71948600	-2.48399800	1.59020300
C	-4.06242100	-2.62331200	0.50440700	H	7.81225300	-3.11563100	2.46907200
H	-5.06943100	-2.98282700	0.67423900	C	8.79515300	-2.34438200	0.70807500
C	-3.85614700	-1.28914800	0.11384800	H	9.72951100	-2.86512000	0.89609800
C	-4.68894300	0.63046200	-1.19779800	C	8.65395700	-1.53192900	-0.41388900
C	-3.34739300	1.01970600	-1.39769000	H	9.47940500	-1.41368500	-1.11004400
C	-3.00312800	1.84970600	-2.48283300	C	7.44986200	-0.86109000	-0.65659400
H	-1.96056800	2.07439800	-2.67347700	H	7.36292500	-0.23520400	-1.53662100
C	-3.98926800	2.34307400	-3.32767200	C	5.01571500	-0.26972200	-0.00368200
H	-3.71074400	2.97739300	-4.16342400	C	5.04483800	0.58997700	-1.30457400
C	-5.32508500	1.99494700	-3.11583900	C	5.50909300	1.91327500	-1.28537900
H	-6.10269000	2.37428500	-3.77127100	H	5.81868700	2.36279600	-0.34823700
C	-5.65954900	1.13748500	-2.06608600	C	5.57973800	2.66920800	-2.45704400
H	-6.69591300	0.85802900	-1.91665600	H	5.94054400	3.69300200	-2.41231700
C	-5.00927700	-0.27086900	0.00477700	C	5.18707500	2.11656600	-3.67614800
C	-6.35926800	-0.99314100	-0.21336000	H	5.23721700	2.70478400	-4.58778000
C	-6.51094900	-1.83294300	-1.33179200	C	4.72729400	0.79968700	-3.70987200
H	-5.67819500	-1.96271100	-2.01602300	H	4.41664900	0.35403600	-4.65059700
C	-7.70759300	-2.50231800	-1.57380800	C	4.65693200	0.04578100	-2.53730300
H	-7.79652800	-3.14540200	-2.44474700	H	4.29327400	-0.97449600	-2.58321900
C	-8.78772400	-2.34983400	-0.69929300	C	4.69839800	0.64400200	1.19056500
H	-9.72178200	-2.87179200	-0.88548300	C	5.67137300	1.15773000	2.05283300
C	-8.65136000	-1.52312600	0.41285800	H	6.70793700	0.88044200	1.90096900
H	-9.48035600	-1.39478500	1.10300300	C	5.33740400	2.01729600	3.10060100
C	-7.44755800	-0.85086700	0.65329100	H	6.11594600	2.40254200	3.75146100
H	-7.36432800	-0.21388400	1.52570400	C	4.00119600	2.36013400	3.31633300
C	-5.04216300	0.60215800	1.29695800	H	3.72304100	2.99653100	4.15058600
C	-4.65804700	0.06878900	2.53572700	C	3.01374800	1.86160500	2.47511900

H	1.97135700	2.08687600	2.66519400	H	-7.81172100	-3.11715600	-2.46788600
C	3.35798100	1.03056100	1.39279000	C	-8.79504400	-2.34471200	-0.70764900
C	2.54292000	-0.84674500	0.09764400	H	-9.72936300	-2.86556000	-0.89555400
C	3.86212500	-1.28951800	-0.09966400	C	-8.65410400	-1.53152700	0.41381700
C	4.06555300	-2.62230300	-0.47987900	H	-9.47971500	-1.41282000	1.10969900
H	5.07143100	-2.98593800	-0.64772400	C	-7.45005800	-0.86054700	0.65637100
C	1.67597100	-3.01778600	-0.48523100	H	-7.36331800	-0.23409400	1.53601500
H	0.84521500	-3.68956700	-0.67443200	C	-5.04486100	0.59016500	1.30448100
C	2.97296100	-3.47927900	-0.66020400	C	-4.65682400	0.04614600	2.53724800
H	3.14765000	-4.50979900	-0.95806100	H	-4.29305600	-0.97408700	2.58325500
C	1.39818900	-1.68304600	-0.10416400	C	-4.72719200	0.80017700	3.70973700
C	-0.00000400	0.46895800	-0.00003400	H	-4.41644400	0.35466300	4.65049200
C	1.17425600	1.20384200	0.27648600	C	-5.18711100	2.11700400	3.67589300
C	1.18868200	2.61419300	0.22256700	H	-5.23725800	2.70532000	4.58746100
H	2.11857000	3.15495900	0.35134300	C	-5.57990600	2.66946900	2.45675100
C	0.00001200	3.31272100	-0.00018900	H	-5.94082200	3.69322000	2.41193100
H	0.00001900	4.39678100	-0.00024900	C	-5.50925600	1.91341200	1.28516600
C	-1.17425700	1.20382500	-0.27663400	H	-5.81895800	2.36279400	0.34799300
C	-1.18866600	2.61418200	-0.22286800	B	-0.00001100	-1.04901600	0.00004600
H	-2.11854700	3.15494500	-0.35170400	DMAC-O_S₀			
C	-2.54293900	-0.84672700	-0.09757500	N	-2.77732000	-0.40153700	-0.10441800
C	-1.39821900	-1.68302200	0.10431100	N	2.08811800	-0.48220100	-0.05532700
C	-1.67601800	-3.01772700	0.48549000	C	0.86430700	-1.17916000	-0.06737000
H	-0.84527100	-3.68950200	0.67475000	C	-1.59823600	-2.54747900	-0.10966900
C	-2.97301500	-3.47919400	0.66048300	H	-2.52972400	-3.09467200	-0.17165400
H	-3.14771800	-4.50969000	0.95841400	C	1.19630200	3.05485200	0.69461400
C	-4.06559600	-2.62222100	0.48007800	H	0.33439400	3.71419300	0.68806100
H	-5.07148300	-2.98583200	0.64792700	C	-4.02143800	1.46354200	-0.98486900
C	-3.86214700	-1.28946600	0.09977600	C	-4.01067000	-0.89681200	0.41401100
C	-4.69840900	0.64392200	-1.19066000	C	-0.34852000	-0.44018600	-0.08391500
C	-3.35798500	1.03044900	-1.39291800	C	-1.63334300	1.75217900	-0.55512300
C	-3.01374000	1.86139200	-2.47532000	C	3.26724700	-1.02335200	-0.65773800
H	-1.97134500	2.08663100	-2.66541500	C	-4.10560500	-1.84223600	1.44245800
C	-4.00118000	2.35986900	-3.31657400	H	-3.20253600	-2.24208400	1.88610500
H	-3.72301600	2.99619000	-4.15088100	C	2.16598700	0.86649600	0.36221700
C	-5.33739500	2.01708600	-3.10079900	C	-2.79344300	0.94305600	-0.53630600
H	-6.11593400	2.40230300	-3.75168000	C	3.41346800	1.32843700	0.84384600
C	-5.67137800	1.15761600	-2.05295600	C	-1.58350600	-1.14488600	-0.08816000
H	-6.70795000	0.88038200	-1.90105500	C	-5.19876800	-0.33908200	-0.08184400
C	-5.01573100	-0.26967900	0.00368500	C	-2.97478300	3.56616000	-1.50812700
C	-6.36591400	-0.99076000	-0.21737800	H	-3.04565100	4.57483000	-1.90278200
C	-6.52226100	-1.81687300	-1.34528800	C	3.18834500	-1.84302400	-1.79251200
H	-5.69305900	-1.93727700	-2.03551200	H	2.21982900	-2.10598200	-2.20016800
C	-7.71916200	-2.48493400	-1.58941900	C	4.52002300	-0.62140300	-0.15874400

C	-0.38900100	-3.23764100	-0.07151800	C	-4.03647400	1.47749900	-0.96920000
H	-0.40478100	-4.32383300	-0.07050400	C	-3.96948600	-0.87765400	0.45635100
C	1.03029800	1.71330600	0.29084400	C	-0.34560800	-0.40046300	-0.07932700
C	-1.75986700	3.06539700	-1.06469200	C	-1.63458500	1.78932400	-0.55270900
H	-0.87152700	3.68351300	-1.13751400	C	3.23900700	-1.00784200	-0.67928700
C	3.52124700	2.67293800	1.19265400	C	-4.04370300	-1.88869900	1.43720700
H	4.46582900	3.05814500	1.55948400	H	-3.12936200	-2.26782300	1.87525900
C	5.67189700	-1.08815100	-0.80177800	C	2.17149100	0.88890800	0.38710300
H	6.64719900	-0.78788000	-0.43685100	C	-2.80693200	0.98003700	-0.53316100
C	-5.35313300	-2.28039600	1.88924500	C	3.41671900	1.31473500	0.87619400
H	-5.40174100	-3.02810500	2.67434000	C	-1.56349600	-1.11237200	-0.07275500
C	2.42323900	3.53915300	1.11982500	C	-5.18482100	-0.32846800	-0.02054100
H	2.53406900	4.57676200	1.42011000	C	-3.03281800	3.57592100	-1.51789100
C	0.83857600	-2.58127000	-0.03466700	H	-3.10737700	4.58878200	-1.90253100
H	1.75731900	-3.15149100	0.01940300	C	3.15217700	-1.82366400	-1.82090700
C	-6.52438700	-1.75790800	1.34091800	H	2.18114900	-2.05277500	-2.24380900
H	-7.49498300	-2.10197000	1.68309800	C	4.49945800	-0.63036700	-0.16903200
C	-4.12065200	2.76079000	-1.45688400	C	-0.39689300	-3.23105100	-0.13846600
H	-5.08508700	3.11591700	-1.80440500	H	-0.41783500	-4.31537500	-0.16030700
C	4.53673600	0.30566200	1.05801100	C	1.03424600	1.74951200	0.29324100
C	-6.44454400	-0.76551300	0.36371300	C	-1.80043800	3.09253500	-1.06371100
H	-7.33106800	-0.30602000	-0.06003600	H	-0.93176300	3.73955500	-1.12354500
C	5.59723600	-1.93495500	-1.90702100	C	3.56636200	2.66728600	1.22103600
H	6.50741000	-2.28944400	-2.38086900	H	4.51773000	3.03455800	1.58589300
C	4.34895300	-2.30786200	-2.40428000	C	5.64320700	-1.11478100	-0.81071700
H	4.27251000	-2.94455300	-3.28053200	H	6.62269600	-0.83642300	-0.43940900
C	4.21414600	-0.52785300	2.33343200	C	-5.27408000	-2.38114600	1.85005500
H	4.18438500	0.12477300	3.21194900	H	-5.30799700	-3.15808500	2.60659100
H	4.98676800	-1.28770500	2.49070900	C	2.48728800	3.55032600	1.11102300
H	3.24945300	-1.03383100	2.25235800	H	2.61901800	4.59313200	1.38820400
C	5.90590000	0.97346100	1.26397800	C	0.82006600	-2.56255400	-0.07121700
H	6.19914200	1.58363100	0.40436200	H	1.74366800	-3.12493200	-0.00601500
H	6.67987700	0.22018300	1.43265000	C	-6.46403800	-1.87052600	1.31312200
H	5.89380200	1.61078600	2.15182000	H	-7.42290700	-2.26213200	1.63563900
B	-0.31351600	1.07879800	-0.11940400	C	-4.16964200	2.77421700	-1.47323500
O	-5.15462000	0.66868000	-1.02264900	H	-5.14492300	3.12052600	-1.79459400
DMAC-O_S1				C	4.52522800	0.27041300	1.06687500
N	-2.76913000	-0.35938800	-0.04113300	C	-6.41692300	-0.83236600	0.38736100
N	2.07687500	-0.46078000	-0.07951000	H	-7.31704700	-0.38809300	-0.02281000
C	0.84833400	-1.14635700	-0.09690300	C	5.55887400	-1.95532800	-1.92185500
C	-1.59901300	-2.51412500	-0.16895800	H	6.46543200	-2.32065400	-2.39447000
H	-2.53848000	-3.04269900	-0.27025700	C	4.30659400	-2.30607700	-2.42816700
C	1.24929800	3.09810600	0.67551600	H	4.22502900	-2.93304500	-3.31097900
H	0.41193400	3.78851000	0.64652800	C	4.19472100	-0.58831800	2.32385900

H	4.17067800	0.04677600	3.21523600	H	-5.31421800	-3.18551200	2.57119800
H	4.95780500	-1.36106900	2.46716200	C	2.50040300	3.55246800	1.08521800
H	3.22319600	-1.07944500	2.23177800	H	2.63388500	4.59637000	1.35689000
C	5.90464300	0.91289500	1.28650500	C	0.80876100	-2.55638600	-0.06315500
H	6.20829700	1.53303900	0.43777700	H	1.72985000	-3.12440200	-0.00619000
H	6.66772500	0.14598600	1.44505900	C	-6.47112700	-1.88334400	1.29173400
H	5.89729500	1.53702100	2.18358300	H	-7.42938700	-2.28002700	1.60951200
B	-0.30783400	1.13317200	-0.10623100	C	-4.17205700	2.78892300	-1.45372100
O	-5.18519600	0.70907800	-0.90734600	H	-5.14630300	3.14264700	-1.76841400
DMAC-O_T₁				C	4.52936800	0.26722500	1.06896300
N	-2.77758600	-0.35210800	-0.03998800	C	-6.42588800	-0.83341200	0.38158000
N	2.08010400	-0.46592000	-0.06834300	H	-7.32607100	-0.38217200	-0.02045200
C	0.84746700	-1.14881000	-0.07763600	C	5.56304800	-1.96221400	-1.91678300
C	-1.60904000	-2.50818100	-0.18377000	H	6.46911800	-2.32801700	-2.39004600
H	-2.54974500	-3.03180000	-0.30006000	C	4.31032600	-2.31115600	-2.42225800
C	1.26165000	3.09726100	0.65508400	H	4.22754600	-2.93795400	-3.30515000
H	0.42438900	3.78778600	0.62468300	C	4.18941300	-0.58120900	2.32983900
C	-4.04369700	1.49384100	-0.94478000	H	4.16613200	0.05927800	3.21745300
C	-3.97912300	-0.87904900	0.45000000	H	4.94788600	-1.35705200	2.48034800
C	-0.34817800	-0.39181200	-0.06551600	H	3.21575100	-1.06776500	2.23739600
C	-1.62438400	1.78663400	-0.54850100	C	5.91033600	0.90532600	1.29025000
C	3.24325200	-1.01664100	-0.67111500	H	6.22017300	1.51908500	0.43908800
C	-4.05056800	-1.90471300	1.41566200	H	6.66950800	0.13607000	1.45607300
H	-3.13564400	-2.28883500	1.84724700	H	5.90234300	1.53489800	2.18362300
C	2.17843500	0.88686700	0.37823800	B	-0.30535200	1.13023500	-0.11043800
C	-2.80896500	0.98361600	-0.51944000	O	-5.19333000	0.73807300	-0.87463700
C	3.42622800	1.31515000	0.86581000	DMAC-S_S₀			
C	-1.56829900	-1.10960800	-0.07188700	N	-2.64322800	-0.41697000	-0.16213300
C	-5.19248400	-0.32169900	-0.01576200	N	2.23039700	-0.46929700	-0.09521600
C	-3.02601600	3.58035200	-1.50353000	C	1.01203700	-1.17365300	-0.14927200
H	-3.09593700	4.59323600	-1.88969900	C	-1.44760200	-2.54509900	-0.23421500
C	3.15593400	-1.82987800	-1.81277400	H	-2.38369600	-3.08695900	-0.29154600
H	2.18453400	-2.06330000	-2.23232100	C	1.30626200	3.00737800	0.87621700
C	4.50322400	-0.64063100	-0.16235300	H	0.43814500	3.65746300	0.91478800
C	-0.41269100	-3.22799700	-0.15319300	C	-3.87653800	1.47575300	-1.05658800
H	-0.43265600	-4.31133600	-0.19631200	C	-3.78036000	-0.93062000	0.54232700
C	1.04701100	1.74975600	0.27949700	C	-0.20334200	-0.44111000	-0.13320200
C	-1.79434100	3.09441500	-1.05690500	C	-1.50958200	1.75840000	-0.48330600
H	-0.92470300	3.73902700	-1.12497700	C	3.41360900	-0.96724800	-0.72539000
C	3.57787000	2.66722700	1.19794400	C	-3.62971500	-1.68031700	1.71858300
H	4.53002700	3.03526100	1.56075200	H	-2.63477600	-1.88537900	2.09545600
C	5.64783800	-1.12359900	-0.80497300	C	2.29540500	0.85249800	0.40265900
H	6.62721200	-0.84454500	-0.43376900	C	-2.66938900	0.94385400	-0.55861600
C	-5.28002700	-2.40047200	1.82335800	C	3.53984900	1.29592500	0.91013300

C	-1.43293300	-1.14562700	-0.17045000	N	-2.62795600	-0.36770900	-0.08799600
C	-5.07722600	-0.62408800	0.10289500	N	2.21780400	-0.44169600	-0.12425400
C	-2.81650800	3.62558200	-1.38198400	C	0.99442900	-1.13400100	-0.17908900
H	-2.87463800	4.65874700	-1.70995500	C	-1.44983500	-2.50408200	-0.29487100
C	3.33978900	-1.72652400	-1.90171700	H	-2.39470300	-3.02470200	-0.39546900
H	2.37294400	-1.97492300	-2.32236400	C	1.36840300	3.04761000	0.88508800
C	4.66337200	-0.58321500	-0.20555300	H	0.52638400	3.73236100	0.90777500
C	-0.23671100	-3.23462600	-0.22937500	C	-3.87942500	1.49618400	-1.05448600
H	-0.24922600	-4.32020600	-0.26515400	C	-3.74314000	-0.92068700	0.56689900
C	1.15134900	1.69299200	0.38699200	C	-0.20140800	-0.39402400	-0.11635700
C	-1.61859000	3.09499800	-0.92365500	C	-1.50245900	1.80307200	-0.46491700
H	-0.72881600	3.71572600	-0.92541300	C	3.38056000	-0.94604300	-0.75534300
C	3.63575100	2.61664000	1.34260700	C	-3.57939900	-1.77375500	1.68100500
H	4.57769800	2.98673600	1.73102500	H	-2.58015300	-1.96826000	2.05088100
C	5.81827400	-1.00533500	-0.87344300	C	2.30546000	0.87493300	0.43372300
H	6.79156700	-0.71743500	-0.49350300	C	-2.67647200	0.98663500	-0.55364400
C	-4.74441700	-2.17734600	2.38949300	C	3.54976400	1.27217900	0.94958100
H	-4.60346200	-2.76940300	3.28838600	C	-1.41442800	-1.10310000	-0.14689800
C	2.52953500	3.47544800	1.32833400	C	-5.05827500	-0.60525900	0.14965600
H	2.63154100	4.49260500	1.69438700	C	-2.85500400	3.65217200	-1.37387700
C	0.98994300	-2.57595000	-0.18032400	H	-2.91917300	4.69180700	-1.68244200
H	1.91061800	-3.14546200	-0.15725100	C	3.29290400	-1.69451100	-1.94297200
C	-6.03138800	-1.90066900	1.92344400	H	2.32143800	-1.89991700	-2.37673600
H	-6.90149600	-2.28380800	2.44693000	C	4.64091200	-0.59461800	-0.22555900
C	-3.95260800	2.81241500	-1.43884500	C	-0.24880800	-3.21782100	-0.31050800
H	-4.89389600	3.20546700	-1.81074100	H	-0.26608900	-4.29997700	-0.38250500
C	4.67338500	0.27316400	1.06184500	C	1.16300000	1.73200400	0.40437800
C	-6.19450200	-1.10267800	0.79351700	C	-1.64987800	3.14177100	-0.89120900
H	-7.18717000	-0.84230200	0.43978800	H	-0.78110300	3.79093700	-0.86071300
C	5.74919700	-1.79223400	-2.02251300	C	3.68975700	2.59622400	1.39382900
H	6.66170400	-2.11329600	-2.51529700	H	4.63943500	2.94281500	1.78239400
C	4.50353700	-2.14880000	-2.53794300	C	5.78418600	-1.03677200	-0.89701800
H	4.43140800	-2.73886000	-3.44657800	H	6.76386400	-0.77820800	-0.51241100
C	4.36128400	-0.63569000	2.28755500	C	-4.67860000	-2.34060600	2.30749500
H	4.32656300	-0.03518800	3.20231600	H	-4.52761200	-2.98896300	3.16452300
H	5.14163100	-1.39562000	2.39973200	C	2.60486400	3.47623800	1.35185300
H	3.40152900	-1.14584100	2.17845100	H	2.72928000	4.49665400	1.70490800
C	6.03668800	0.94092000	1.30405700	C	0.97030400	-2.54840600	-0.22789600
H	6.32182100	1.60340900	0.48124500	H	1.89539500	-3.11154100	-0.20020700
H	6.81814700	0.18646000	1.42634400	C	-5.97527300	-2.05730600	1.85779400
H	6.02124500	1.52448800	2.22806800	H	-6.83586200	-2.49656700	2.35151900
B	-0.18535000	1.07585200	-0.06884200	C	-3.98026800	2.83745500	-1.46514200
S	-5.27249700	0.39983500	-1.33931600	H	-4.92722700	3.22101100	-1.82878000
DMAC-S₁				C	4.66686600	0.22609800	1.06430100

C	-6.15930100	-1.17997700	0.79468900	C	-1.64871100	3.14911200	-0.87726400
H	-7.15950900	-0.92504100	0.45902400	H	-0.77736300	3.79507000	-0.85863900
C	5.69932200	-1.81027900	-2.05611500	C	3.70649700	2.60103300	1.36419400
H	6.60599500	-2.14288300	-2.55197700	H	4.65659000	2.94877400	1.75075400
C	4.44729900	-2.13563500	-2.58001600	C	5.78637900	-1.06509500	-0.88767600
H	4.36630700	-2.70916000	-3.49835300	H	6.76732700	-0.81116700	-0.50339200
C	4.34913300	-0.71476600	2.26507300	C	-4.69046700	-2.35481100	2.29203300
H	4.32562700	-0.13874500	3.19563300	H	-4.54079800	-3.00345400	3.14896400
H	5.11837900	-1.48943400	2.35402600	C	2.62130300	3.48359300	1.31986300
H	3.38050800	-1.20603800	2.14632900	H	2.74883000	4.50551200	1.66728300
C	6.04340600	0.86264900	1.31759000	C	0.96474900	-2.53782500	-0.21212800
H	6.33681200	1.54032100	0.51032700	H	1.88888000	-3.10300800	-0.18473700
H	6.81258700	0.09235300	1.41956300	C	-5.98473500	-2.08349000	1.82990800
H	6.03847200	1.42478400	2.25466100	H	-6.84586700	-2.53266400	2.31373800
B	-0.18062000	1.13618200	-0.04022100	C	-3.98642700	2.84921600	-1.43256400
S	-5.31790400	0.46686700	-1.22795800	H	-4.93242500	3.23758400	-1.79325900
DMAC-S_T₁				C	4.67533800	0.22713400	1.05816200
N	-2.63350000	-0.35882400	-0.08278800	C	-6.16762400	-1.20416900	0.76816200
N	2.22126400	-0.43963500	-0.12171100	H	-7.16720600	-0.95546700	0.42602200
C	0.99402100	-1.12924900	-0.16598700	C	5.69689000	-1.84385500	-2.04252700
C	-1.45387100	-2.49286000	-0.29202100	H	6.60163400	-2.18655900	-2.53500000
H	-2.40000000	-3.01126900	-0.39497300	C	4.44351700	-2.16082000	-2.56742900
C	1.38338300	3.05486500	0.86071000	H	4.35928100	-2.73817800	-3.48298600
H	0.54294900	3.74135700	0.88388600	C	4.35242100	-0.69636700	2.27075600
C	-3.88964700	1.51121800	-1.02556300	H	4.33221900	-0.10851500	3.19391700
C	-3.75487700	-0.92478500	0.56227900	H	5.11787000	-1.47348900	2.36924800
C	-0.20248100	-0.37765900	-0.10890100	H	3.38145900	-1.18449700	2.15867700
C	-1.50029800	1.80843200	-0.45218700	C	6.05479100	0.86041700	1.30330800
C	3.38418400	-0.95632800	-0.74985200	H	6.35124400	1.52640700	0.48750800
C	-3.59078600	-1.77628000	1.67498900	H	6.82026500	0.08787700	1.41505400
H	-2.59248400	-1.96372500	2.05087900	H	6.05274900	1.43423400	2.23325800
C	2.31475200	0.87882600	0.41927600	B	-0.17722800	1.13910000	-0.04289200
C	-2.68029700	0.99480700	-0.53121700	S	-5.32186100	0.47987400	-1.22439700
C	3.56355600	1.27759500	0.93063800	DMAC-Se_S₀			
C	-1.41945100	-1.09310600	-0.14306400	N	-2.30030900	-0.45557900	-0.03053900
C	-5.06560000	-0.61648100	0.13599800	N	2.57568000	-0.46237700	-0.10799300
C	-2.85399400	3.66057800	-1.34936800	C	1.36230200	-1.17686800	-0.14333900
H	-2.91745300	4.69974800	-1.66009800	C	-1.08809600	-2.56703600	-0.17670400
C	3.29137400	-1.70826700	-1.93342400	H	-2.02282400	-3.11373900	-0.21007000
H	2.31861200	-1.91030600	-2.36557700	C	1.64941500	2.97727700	0.98763900
C	4.64491800	-0.60965600	-0.22135700	H	0.77665900	3.61676900	1.07195100
C	-0.25751400	-3.21125500	-0.30373900	C	-3.56229100	1.44343800	-0.88145700
H	-0.27486900	-4.29252800	-0.38109700	C	-3.37390200	-0.98025200	0.76545000
C	1.17372600	1.73786100	0.38880400	C	0.14237800	-0.45574700	-0.07510800

C	-1.19488600	1.73811500	-0.32744300	C	6.41117600	0.95087400	1.20633400
C	3.74294800	-0.93299900	-0.78654000	H	6.66267500	1.63770900	0.39256600
C	-3.10967500	-1.67122300	1.95810100	H	7.20359800	0.20188000	1.28310600
H	-2.08298100	-1.81486500	2.27393200	H	6.42031700	1.50976900	2.14556700
C	2.64362300	0.84638700	0.42272600	B	0.14730400	1.05866000	0.03334300
C	-2.34944100	0.91455900	-0.40124100	Se	-5.04587800	0.26875900	-1.17148800
C	3.89939300	1.28921200	0.90246500	DMAC-Se_S1			
C	-1.08163600	-1.16912100	-0.09054300	N	-2.27726900	-0.41052500	0.04046800
C	-4.70816900	-0.76095900	0.39888800	N	2.56685500	-0.43286400	-0.13865600
C	-2.53381500	3.61439300	-1.15708300	C	1.34917100	-1.13679900	-0.17772700
H	-2.60762400	4.65579500	-1.45472300	C	-1.08580300	-2.52685300	-0.25223000
C	3.63892700	-1.66551900	-1.97747600	H	-2.03006200	-3.05261600	-0.33146700
H	2.66155900	-1.91384200	-2.37312000	C	1.71236700	3.01284800	1.00827100
C	5.00494900	-0.54909000	-0.29708200	H	0.86424300	3.68671000	1.07897300
C	0.12759400	-3.24667600	-0.22419900	C	-3.55971700	1.46341100	-0.88245900
H	0.12277800	-4.33152100	-0.27918200	C	-3.33817300	-0.99005600	0.76513600
C	1.49154000	1.67543300	0.46671700	C	0.14915300	-0.41052200	-0.05927900
C	-1.32317900	3.08355400	-0.73219800	C	-1.18354400	1.77959900	-0.30536000
H	-0.43920000	3.71257000	-0.73306000	C	3.71476400	-0.90576900	-0.81848500
C	3.99622600	2.59847000	1.36815500	C	-3.06859600	-1.80218600	1.88995300
H	4.94655800	2.96765200	1.73645400	H	-2.04098100	-1.93805400	2.20454300
C	6.14193600	-0.94371000	-1.01089600	C	2.65782800	0.86700800	0.45756500
H	7.12408800	-0.65527600	-0.65493100	C	-2.35277900	0.95360600	-0.39694200
C	-4.15174200	-2.18557900	2.72500300	C	3.91311900	1.26180800	0.94815100
H	-3.92381200	-2.72936100	3.63652200	C	-1.05748000	-1.12915200	-0.07374200
C	2.88187200	3.44563600	1.41352500	C	-4.68698000	-0.76092400	0.41231300
H	2.98578000	4.45324300	1.80459000	C	-2.56637300	3.64237800	-1.13730200
C	1.35015600	-2.57838300	-0.20348200	H	-2.64656800	4.69085100	-1.41044200
H	2.27562200	-3.14035700	-0.22192000	C	3.59856300	-1.62151300	-2.02383200
C	-5.47862100	-1.98617400	2.33718500	H	2.61638900	-1.82542600	-2.43348100
H	-6.29341400	-2.38068900	2.93602000	C	4.98718200	-0.55610000	-0.31691900
C	-3.65994100	2.78895700	-1.22241000	C	0.12013000	-3.22824200	-0.32469900
H	-4.60944200	3.18368300	-1.57111100	H	0.11053500	-4.30845600	-0.42285800
C	5.04732600	0.27508400	0.99076400	C	1.50626200	1.71178800	0.49061300
C	-5.75241900	-1.25134100	1.18618500	C	-1.35046100	3.12966700	-0.68679200
H	-6.77868900	-1.05315700	0.89313000	H	-0.48741100	3.78602100	-0.64778000
C	6.04380600	-1.70400700	-2.17567200	C	4.05277300	2.57235700	1.43111900
H	6.94319100	-2.00422100	-2.70441000	H	5.01031100	2.91711400	1.80160400
C	4.78581100	-2.06116100	-2.65978900	C	6.11381600	-0.96654000	-1.03496600
H	4.69040900	-2.63072800	-3.57929100	H	7.10214000	-0.70870600	-0.67265700
C	4.78409100	-0.66829900	2.20181700	C	-4.09925600	-2.40027000	2.59777200
H	4.77285700	-0.09193900	3.13257300	H	-3.86677500	-3.01326500	3.46262000
H	5.57522200	-1.42237600	2.26910100	C	2.95804600	3.44052200	1.45141100
H	3.82647200	-1.18587400	2.11015600	H	3.08236500	4.45024600	1.83400500

C	1.33585400	-2.54912800	-0.26432800	H	-2.65837800	4.69781600	-1.37899700
H	2.26621800	-3.10405000	-0.28084300	C	3.58813900	-1.64931400	-2.00657700
C	-5.43235100	-2.19211200	2.21885100	H	2.60316700	-1.84875500	-2.41123400
H	-6.24078800	-2.65387800	2.77623700	C	4.98908100	-0.57256000	-0.31650200
C	-3.68124600	2.81537800	-1.24563500	C	0.11707100	-3.22473800	-0.28033100
H	-4.63443200	3.20088500	-1.59066100	H	0.10840700	-4.30533100	-0.36722900
C	5.04434900	0.22580400	0.99577200	C	1.51434100	1.72174800	0.47067600
C	-5.71844100	-1.36121500	1.14144500	C	-1.35683300	3.13963300	-0.66823800
H	-6.74879600	-1.16765000	0.86005200	H	-0.49335400	3.79584600	-0.64043500
C	6.00146700	-1.70759100	-2.21279000	C	4.06972300	2.58466600	1.39122400
H	6.89592100	-2.01612500	-2.74507100	H	5.02768500	2.93239900	1.75747300
C	4.73736200	-2.03170000	-2.70776500	C	6.11108000	-1.00697200	-1.02765600
H	4.63423200	-2.57996000	-3.63922500	H	7.10230500	-0.75412800	-0.67018900
C	4.77412800	-0.75475800	2.17632400	C	-4.11707300	-2.37455100	2.61406600
H	4.77269400	-0.20745000	3.12436000	H	-3.88771500	-2.97265600	3.49007200
H	5.55425200	-1.52250100	2.21816600	C	2.97335600	3.45430300	1.40874900
H	3.80780000	-1.25377000	2.07193100	H	3.10061500	4.46667100	1.78320700
C	6.42132300	0.87020200	1.22594000	C	1.33441500	-2.53866000	-0.22424200
H	6.68203100	1.57564600	0.43135300	H	2.26552600	-3.09289300	-0.23317700
H	7.20145200	0.10612100	1.28010300	C	-5.44574300	-2.18651100	2.21576600
H	6.43982500	1.40322300	2.17968800	H	-6.25648300	-2.64857300	2.76977400
B	0.15545800	1.11603100	0.06543800	C	-3.69241300	2.81916600	-1.21188100
Se	-5.08669800	0.34026400	-1.07427400	H	-4.64522700	3.20589400	-1.55649100
DMAC-Se_T₁				C	5.05550500	0.23491000	0.97994900
N	-2.28268000	-0.40482800	0.04230100	C	-5.72787900	-1.37347600	1.12240700
N	2.56853200	-0.42705600	-0.13765700	H	-6.75687300	-1.19178900	0.82841800
C	1.34782100	-1.13008100	-0.15856000	C	5.98943100	-1.76343500	-2.19465500
C	-1.08528300	-2.51847800	-0.22063800	H	6.88030900	-2.08888200	-2.72273800
H	-2.03019000	-3.04460400	-0.29314000	C	4.72226100	-2.07993600	-2.68601500
C	1.72575000	3.02588300	0.97561800	H	4.61312600	-2.63927800	-3.60998000
H	0.87977000	3.70205100	1.04618700	C	4.78802000	-0.72176400	2.18072100
C	-3.56936600	1.47003000	-0.86088000	H	4.79413800	-0.15627900	3.11786200
C	-3.35185700	-0.98941200	0.76721800	H	5.56593500	-1.49091600	2.23251300
C	0.14683900	-0.39186600	-0.05078500	H	3.81954000	-1.21964900	2.09191500
C	-1.18554100	1.78692500	-0.29099300	C	6.43573800	0.87936000	1.18997100
C	3.71445500	-0.91931700	-0.81173800	H	6.69356600	1.56913300	0.38089900
C	-3.08380400	-1.77522600	1.90684100	H	7.21379700	0.11408900	1.25396500
H	-2.05789000	-1.89658500	2.23321900	H	6.46169600	1.42949600	2.13365100
C	2.66650800	0.87621900	0.43881900	B	0.15640300	1.12188800	0.06084000
C	-2.35622500	0.95985400	-0.37743600	Se	-5.07682400	0.32526400	-1.10029900
C	3.92755700	1.27388100	0.92034000	BN-O-Se_S₀			
C	-1.06294800	-1.11836600	-0.06142400	N	-1.95779800	-0.46971000	-0.02949000
C	-4.69367000	-0.77589000	0.39594800	N	2.91490700	-0.41438400	0.06951200
C	-2.57419400	3.64926000	-1.10677900	C	1.71777200	-1.14864700	0.00183300

C	-0.71556800	-2.56321800	-0.12600900	C	5.49993500	-2.21106500	-1.98622600
H	-1.64200300	-3.11970600	-0.19949600	H	5.55211200	-2.92027500	-2.80598300
C	1.90453100	3.00360300	1.20326300	B	0.45910700	1.07726400	0.14559400
H	1.01802400	3.62123300	1.30066800	Se	-4.66141700	0.22453500	-1.28399800
C	-3.21322500	1.41979300	-0.91179900	O	5.28974700	0.59651800	1.06158100
C	-3.05796200	-1.01735300	0.71479000	BN-O-Se_S1			
C	0.48723400	-0.43628200	0.01887300	N	-1.94543300	-0.44708300	0.00784000
C	-0.87779000	1.74256900	-0.25112500	N	2.90776800	-0.37117800	0.00952100
C	4.15140000	-0.89141100	-0.45951000	C	1.69700400	-1.11846400	-0.00332000
C	-2.83631200	-1.71027900	1.91483300	C	-0.70008300	-2.54834500	-0.07358900
H	-1.82280300	-1.83926600	2.27624500	H	-1.63155700	-3.09609100	-0.15622900
C	2.93326900	0.90504900	0.57141100	C	1.95162100	3.02496700	1.21452700
C	-2.01403900	0.90320700	-0.38639200	H	1.08532100	3.67206700	1.30377800
C	4.16037300	1.39669300	1.05495100	C	-3.20438300	1.40741500	-0.95682000
C	-0.72799600	-1.16505300	-0.04363300	C	-3.03717000	-0.99795800	0.73750900
C	-4.37756400	-0.81577600	0.29010800	C	0.48345300	-0.39918400	0.03139400
C	-2.20985700	3.61208700	-1.10381600	C	-0.87355800	1.77694300	-0.25186100
H	-2.28886500	4.65758100	-1.38521000	C	4.10838200	-0.87181100	-0.50410500
C	4.25061100	-1.78698300	-1.53115300	C	-2.81726800	-1.70232800	1.93568600
H	3.34976200	-2.15866700	-2.00297300	H	-1.80555800	-1.80799400	2.31013400
C	5.33730400	-0.36551300	0.07422400	C	2.95022200	0.94022900	0.57174000
C	0.50695400	-3.23063500	-0.10984100	C	-2.01293900	0.92283300	-0.41290000
H	0.51543300	-4.31595200	-0.15280800	C	4.18015200	1.40723600	1.04086800
C	1.77645200	1.71838100	0.62653100	C	-0.71323300	-1.13485500	0.00283100
C	-1.01009100	3.09368300	-0.63522200	C	-4.36031600	-0.81189000	0.30066100
H	-0.13750000	3.73656300	-0.58402900	C	-2.26640800	3.62517600	-1.09471400
C	4.26076800	2.66711400	1.59447100	H	-2.36764800	4.67702700	-1.34827100
H	5.22409000	2.99905800	1.96703500	C	4.18322300	-1.83547100	-1.53145800
C	6.58498700	-0.77815100	-0.37883800	H	3.26974900	-2.18815100	-1.99270100
H	7.46992700	-0.34523000	0.07506200	C	5.32412000	-0.35377800	0.00583100
C	-3.90335600	-2.24560100	2.63136700	C	0.51088100	-3.22816000	-0.03283900
H	-3.70792200	-2.79060800	3.54963300	H	0.52434700	-4.31257800	-0.05447300
C	3.11829000	3.47489600	1.67967000	C	1.78411900	1.75414200	0.63170100
H	3.19151300	4.46151000	2.12608700	C	-1.05930400	3.13824500	-0.60905100
C	1.72106300	-2.55104500	-0.04034200	H	-0.21374300	3.81401400	-0.52590200
H	2.64805100	-3.10774300	0.00201800	C	4.31585100	2.67317500	1.61785000
C	-5.21443600	-2.06547500	2.18478700	H	5.29125700	2.99553300	1.96302400
H	-6.04884600	-2.47645500	2.74421100	C	6.55623900	-0.84465300	-0.41795800
C	-3.31758900	2.76926000	-1.23475000	H	7.45609100	-0.42579200	0.01862400
H	-4.25691000	3.15490700	-1.61925700	C	-3.88149100	-2.25586500	2.63954000
C	-5.44812800	-1.32781400	1.02684200	H	-3.68749000	-2.80071000	3.55827200
H	-6.46327300	-1.14331400	0.68958500	C	3.18409100	3.47715100	1.70230100
C	6.66857500	-1.72293300	-1.40178500	H	3.26139900	4.46639100	2.14332900
H	7.64050300	-2.05622300	-1.75070700	C	1.71972000	-2.52217600	0.02723100

H	2.65431000	-3.06349000	0.10411700	C	4.31244100	2.69768000	1.59319700
C	-5.19206600	-2.08790000	2.18312700	H	5.28659300	3.03048100	1.93003900
H	-6.02583400	-2.51096200	2.73451100	C	6.56478200	-0.84110800	-0.40676600
C	-3.35161500	2.76384800	-1.27730800	H	7.46397900	-0.41174100	0.02043600
H	-4.29620600	3.12932400	-1.66539300	C	-3.87107600	-2.22559100	2.65983000
C	-5.42654100	-1.34608800	1.02746000	H	-3.67179300	-2.75684000	3.58547900
H	-6.44195000	-1.17743000	0.68251700	C	3.17010200	3.48854000	1.67827000
C	6.60316600	-1.83682000	-1.39228500	H	3.24055500	4.47975100	2.11670900
H	7.56167200	-2.21813100	-1.72781700	C	1.73219500	-2.51739000	0.04855100
C	5.41338800	-2.31410000	-1.96019100	H	2.66841900	-3.05254300	0.14719700
H	5.44779400	-3.05378800	-2.75311000	C	-5.18394400	-2.06324300	2.20974400
B	0.45416600	1.13163600	0.14285100	H	-6.01475900	-2.47629700	2.77317600
Se	-4.65032800	0.19507300	-1.29010700	C	-3.37040000	2.75692800	-1.25904500
O	5.32580800	0.64110300	0.94028800	H	-4.31696700	3.12201800	-1.64354900
BN-O-Se_T1				C	-5.42417100	-1.34089900	1.04290800
N	-1.95035800	-0.45856400	-0.01896400	H	-6.44113300	-1.17447700	0.70136800
N	2.91526200	-0.36210700	0.00942600	C	6.61092100	-1.85012300	-1.36082000
C	1.70089700	-1.11653900	-0.00535600	H	7.56924000	-2.23734900	-1.68966200
C	-0.68550100	-2.54550800	-0.08408800	C	5.42052100	-2.33845200	-1.92247200
H	-1.61394500	-3.10055000	-0.15763700	H	5.45694700	-3.09002600	-2.70371900
C	1.93841200	3.03009400	1.19886000	B	0.44880400	1.12728100	0.13958000
H	1.07093700	3.67458100	1.29268000	Se	-4.64864100	0.17259100	-1.30011200
C	-3.21864000	1.40181700	-0.95192700	O	5.33099200	0.68175400	0.90440000
C	-3.03614400	-1.00391000	0.73178100	<hr/>			
C	0.48520100	-0.39196000	0.00954900				
C	-0.89187800	1.77431700	-0.24692300				
C	4.11707800	-0.87178700	-0.49415800				
C	-2.80943700	-1.68575900	1.93946700				
H	-1.79516300	-1.79221300	2.30680800				
C	2.94832500	0.94666000	0.55700500				
C	-2.02216300	0.91730900	-0.41243300				
C	4.18255200	1.43103800	1.01363700				
C	-0.71225100	-1.13999400	-0.02671300				
C	-4.35990400	-0.82400700	0.30084300				
C	-2.28729800	3.62156000	-1.07901700				
H	-2.39160500	4.67371700	-1.32955600				
C	4.19070700	-1.85653600	-1.50205700				
H	3.27738200	-2.21767300	-1.95596900				
C	5.33033900	-0.34067300	0.00297600				
C	0.52989500	-3.22761100	-0.01184900				
H	0.54352800	-4.31190600	-0.00643100				
C	1.76695600	1.75184700	0.62288700				
C	-1.07735200	3.13298600	-0.60080700				
H	-0.23172300	3.80911000	-0.52039100				