

Supporting Information

The combination of skeleton-engineering and periphery-engineering: a design strategy for organic doublet emitters

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Details on the spin-orbit coupling (SOC) matrix elements calculations

The spin-orbit couplings (SOC) matrix elements are calculated using Quasi-degenerate strongly contracted N-electron valence state second-order perturbation theory QD-SC-NEVPT2(5,6)/Def2-TZVP, which are defined as

$$\text{SOC} = \langle D_1 | \hat{H}_{\text{soc}} | Q_1 \rangle \quad (1.11)$$

here, \hat{H}_{soc} is the spin-orbit couplings Hamiltonian operator.

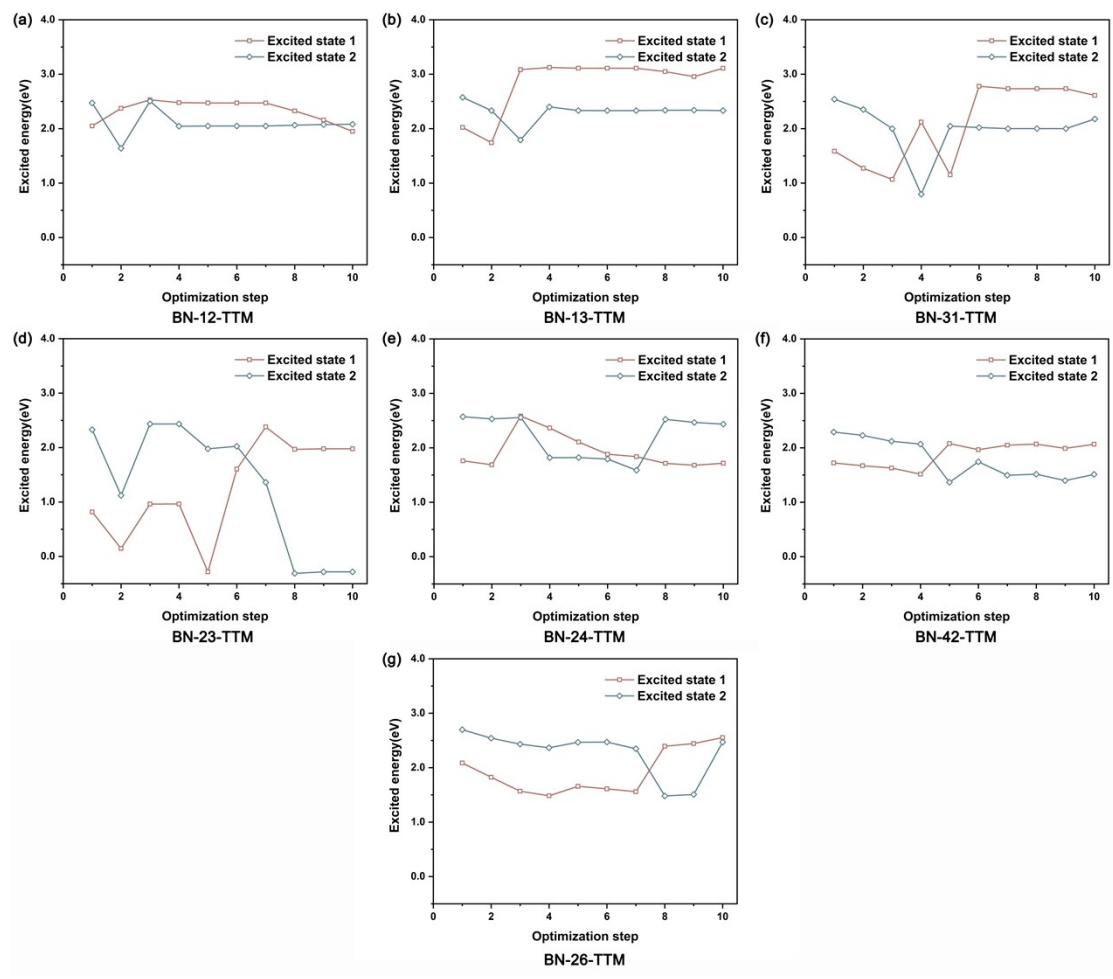


Fig. S1. Potential energy curves showing D_2/D_1 conical intersections (CI) along the relaxation process from D_1 to D_0 structure.

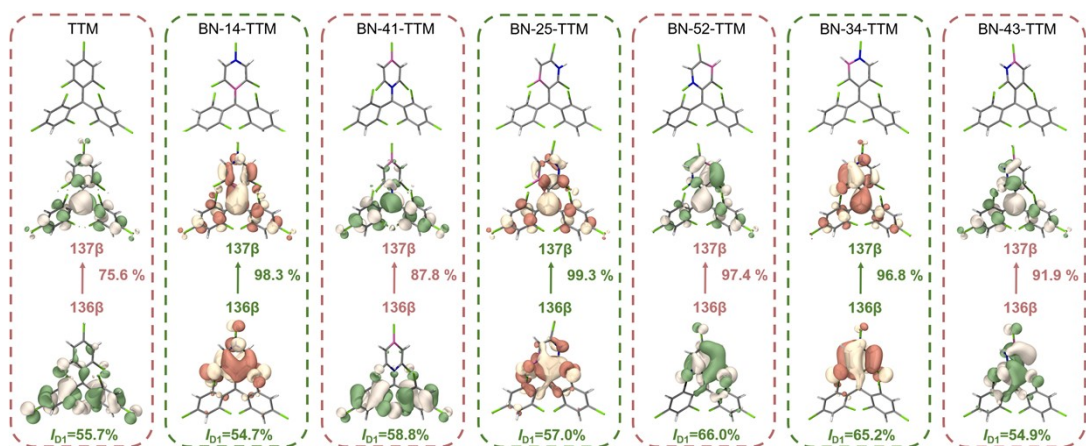


Fig. S2. Natural transition orbitals (NTO) analysis for D_1 to D_0 states of TTM and orientational isomers.

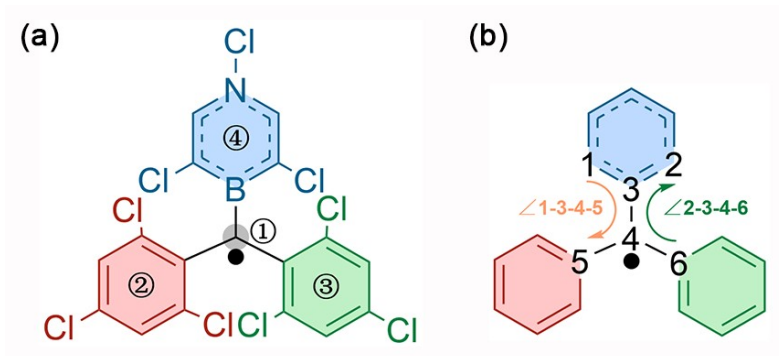


Fig. S3. (a) Fragment definition; (b) Selected dihedral angles definition, the dihedral angles in orange and green present $\angle 1-3-4-5$ and $\angle 2-3-4-6$, respectively.

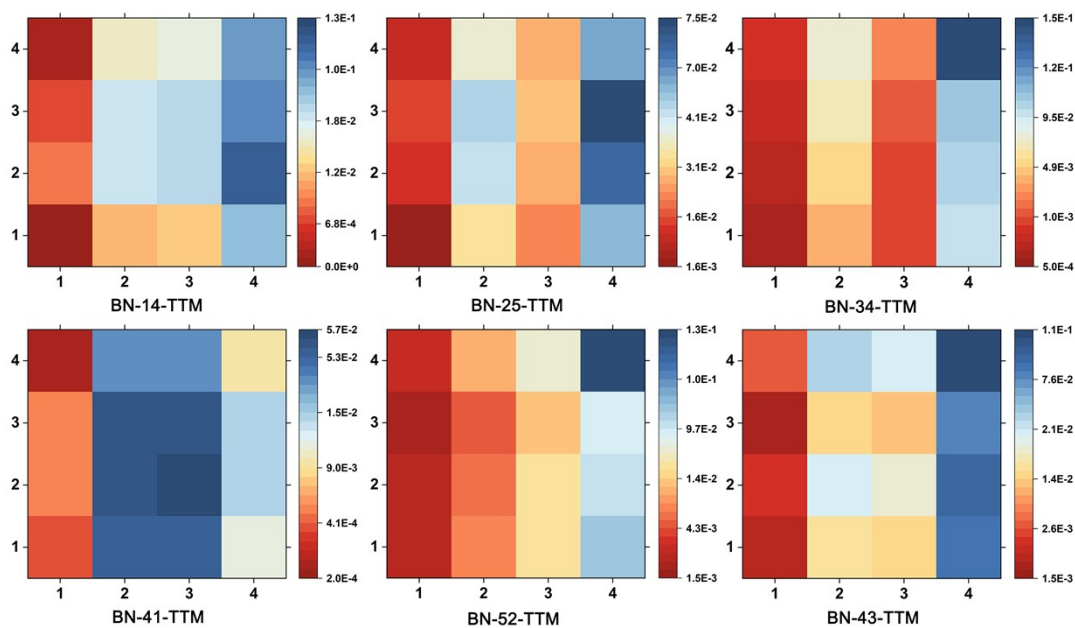


Fig. S4. Fragment-based transition density matrix (TDM) heat map of orientational isomers for D_1 to D_0 states.

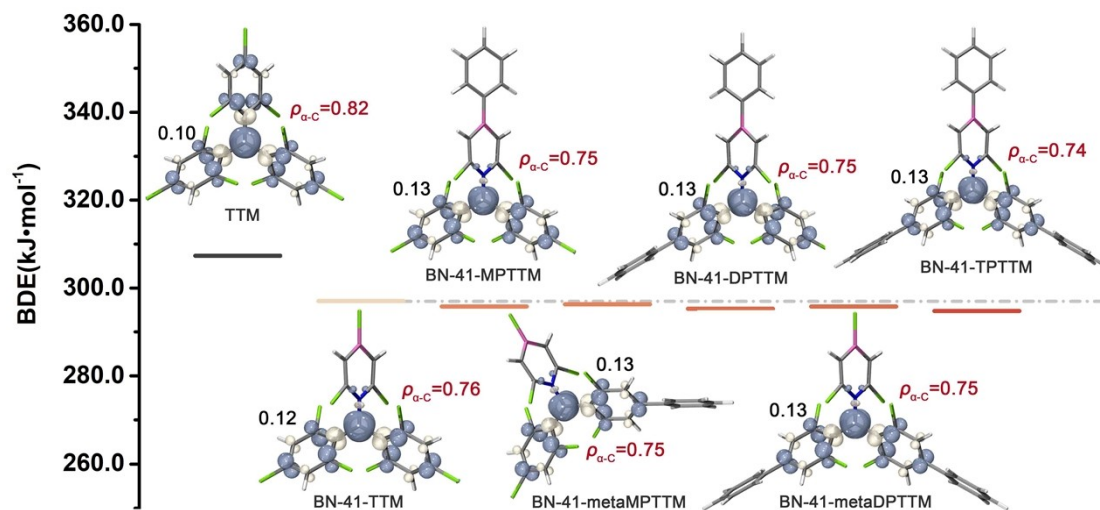


Fig. S5. Calculated Bond dissociation energy (BDE) of radicals' precursors, spin-density, and spin-population of radicals.

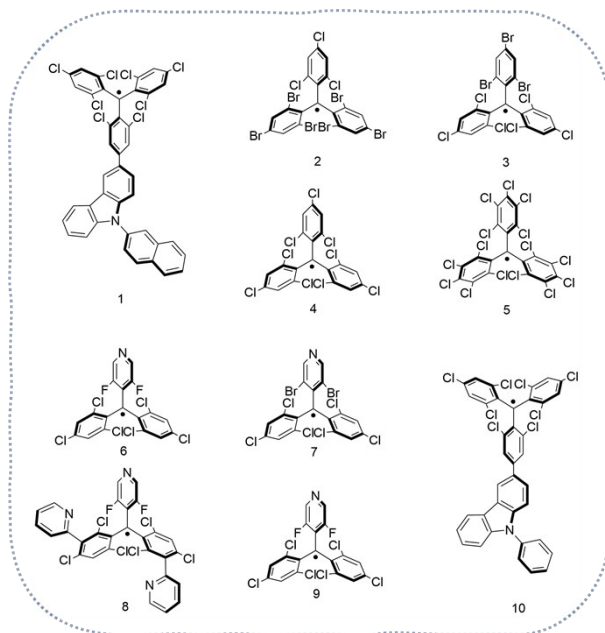


Fig. S6. The molecular structures of the studied radicals.

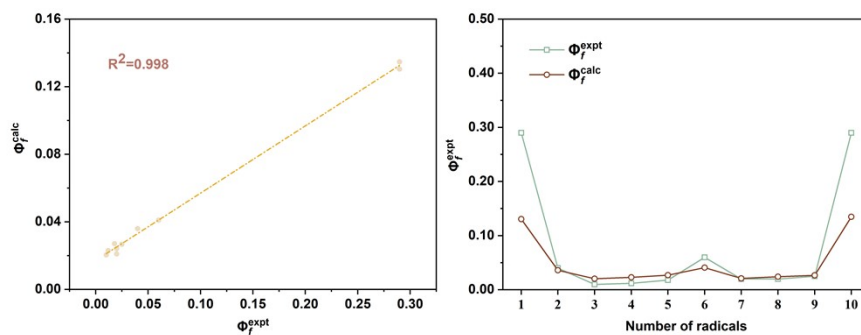


Fig. S7. The correlations of experimental and calculated photoluminescence quantum yield (Φ_{pl}) for each radical.

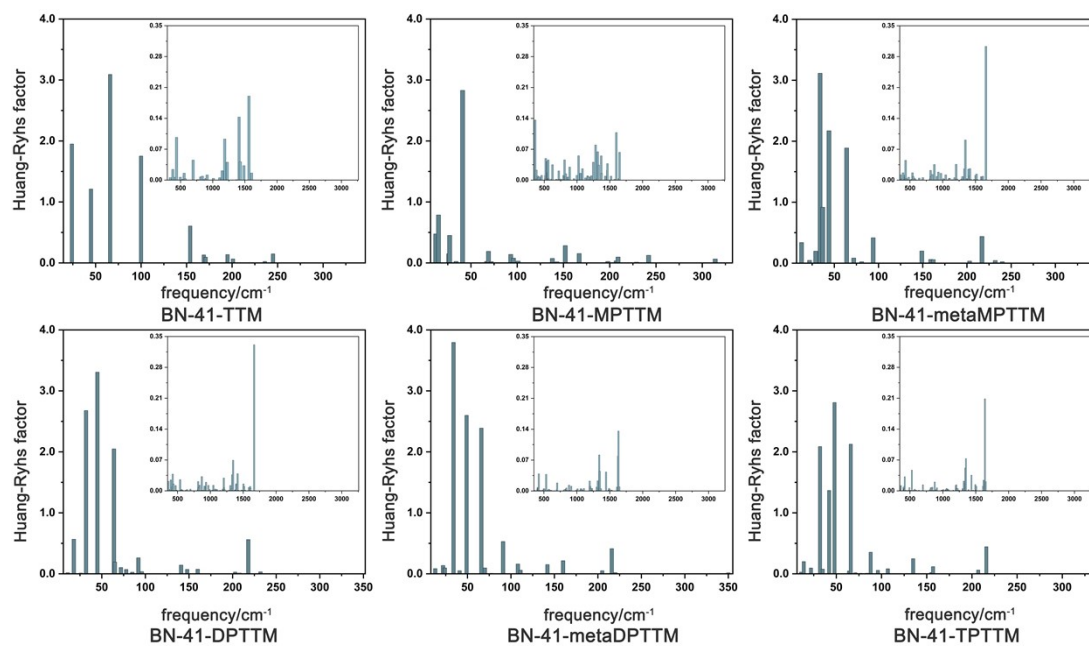


Fig. S8. The effective Huang-Rhys factor (S_{eff}) versus the frequency in the D_1 state. Inset: the HR factors of high-frequency modes.

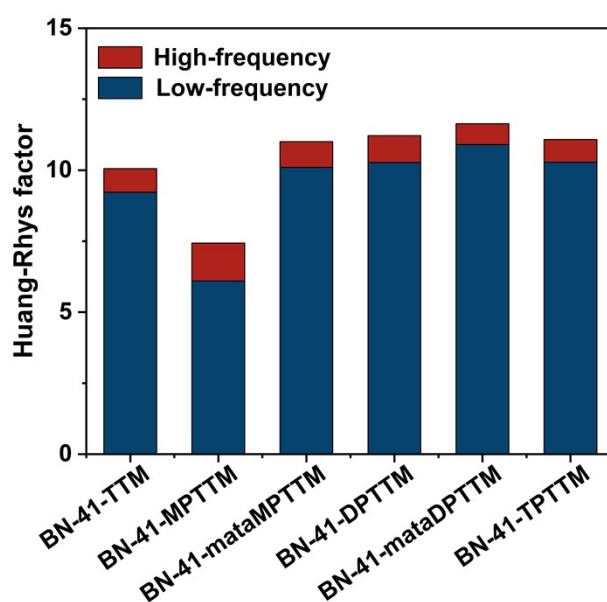


Fig. S9. Calculated effective HR factor (S_{eff}) corresponding to low-frequency modes and total HR factor of high-frequency modes.

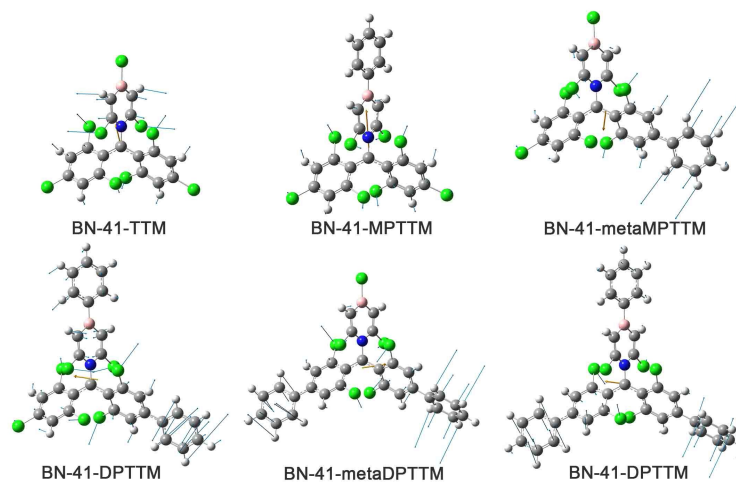


Fig. S10. Diagrammatic illustrations of the displacement vectors for the representative low-frequency vibrational normal modes.

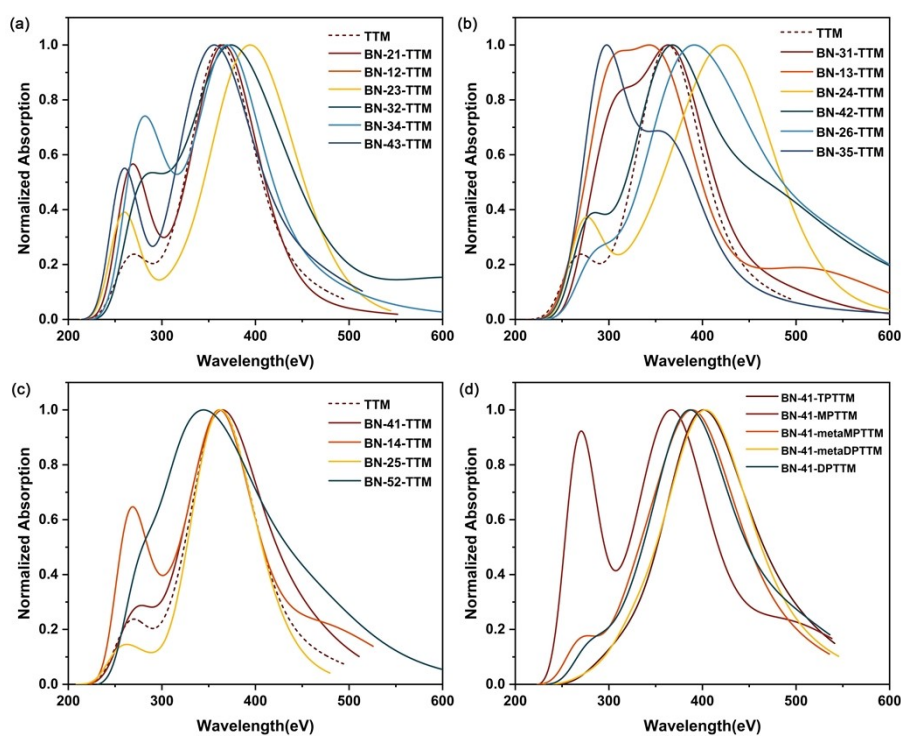


Fig. S11. Normalized absorption spectra computed at the UPBE0/6-311G(d,p) level in cyclohexane: (a) skeleton-engineered radicals in ortho-substitution; (b) skeleton-engineered radicals in meta-substitution; (c) skeleton-engineered radicals in para-substitution; (d) periphery-engineered radicals.

Table S1. Excitation energies (eV) of TTM and BN-41-TTM computed using QD-SC- NEVPT2 (5,6)/Def2-TZVP.

	λ_{abs} (eV)		λ_{emi} (eV)	
	Expt.	Calc.	Expt.	Calc.
TTM	3.34	3.24	2.20	2.16
BN-41-TTM	/	/	2.26 ^a	2.36

^a The data of spin-unrestricted TD-DFT using PBE0/6-311G(d,p) level.

Table S2. The emission energies (E), emission wavelengths (λ_{emi}), oscillator strengths (f), and the radiative decay rate (k_r) of radicals without CI phenomenon.

	E (eV)	λ_{emi} (nm)	f	k_r ($\times 10^6$ s ⁻¹)
BN-21-TTM	1.61	772	0.0083	0.9
BN-14-TTM	1.76	706	0.0421	5.6
BN-41-TTM	2.26	549	0.0286	6.3
BN-23-TTM	2.07	600	0.0145	2.7
BN-32-TTM	1.52	814	0.0657	6.6
BN-25-TTM	2.16	575	0.0241	4.9
BN-52-TTM	1.44	861	0.0191	1.7
BN-34-TTM	1.44	862	0.0145	1.3
BN-43-TTM	2.05	605	0.0362	6.6

Table S3. Selected bond lengths (the bonds between α -C and other groups, Å) in D_0 or D_1 states and the changes between these two states (Å) of orientational isomers.

	Bond 1			Bond 2			Bond 3		
	D_0	D_1	Δ	D_0	D_1	Δ	D_0	D_1	Δ
BN-14-TTM	1.562	1.486	-0.076	1.463	1.447	-0.015	1.463	1.448	-0.016
BN-41-TTM	1.426	1.426	0.000	1.455	1.427	-0.027	1.455	1.428	-0.027
BN-25-TTM	1.456	1.446	-0.010	1.467	1.438	-0.029	1.468	1.445	-0.023
BN-52-TTM	1.463	1.415	-0.048	1.464	1.461	-0.003	1.461	1.448	-0.013
BN-34-TTM	1.467	1.406	-0.061	1.466	1.460	-0.006	1.464	1.465	0.001
BN-43-TTM	1.464	1.456	-0.008	1.464	1.436	-0.028	1.464	1.450	-0.014

Table S4. Selected dihedral angles ($^\circ$) in D_0 or D_1 states with their difference Δ (D_1 - D_0) ($^\circ$).

	$\angle 1-3-4-5$			$\angle 2-3-4-6$		
	D_0	D_1	Δ (D_1 - D_0)	D_0	D_1	Δ (D_1 - D_0)
BN-14-TTM	42.49	34.72	-7.77	42.65	35.13	-7.52
BN-41-TTM	57.97	60.19	2.22	58.06	60.15	2.09
BN-25-TTM	44.45	46.96	2.51	44.24	45.41	1.17
BN-52-TTM	47.37	42.34	-5.03	49.36	38.01	-11.35
BN-34-TTM	48.21	31.02	-17.19	48.18	33.47	-14.71
BN-43-TTM	50.19	52.10	1.91	50.01	53.44	3.43

Table S5. Detailed data on interfragment electron redistribution (IER) and net transferred electrons between fragments (the number represents the fragment number).

	BN-41-TTM	BN-41-MPTTM	BN-41-metaMPTTM	BN-41-DPTTM	BN-41-metaDPTTM	BN-41-TPTTM
IER₁	0.00903	0.00776	0.01469	0.01671	0.01304	0.01439
IER₂	0.12867	0.00311	0.39034	0.40696	0.13453	0.20650
IER₃	0.12872	0.00675	0.01794	0.01940	0.17647	0.09848
IER₄	0.00793	0.09179	0.00478	0.00329	0.00196	0.00514
Net 1→2	-0.13692	0.00037	-0.16210	-0.14031	-0.09300	-0.11184
Net 1→3	-0.13700	-0.00456	-0.01575	-0.01615	-0.11459	-0.06197
Net 1→4	-0.02725	-0.36117	-0.01327	-0.00653	-0.00486	-0.01175
Net 2→3	-0.00009	-0.00325	0.08014	0.06104	-0.01700	0.04264
Net 2→4	0.01242	-0.23758	0.01777	0.02572	0.01673	0.01716
Net 3→4	0.01245	-0.24582	-0.00483	0.00012	0.02150	0.00503

Table S6. The excitation energies of D_1 (E_D /a.u.), Q_1 (E_Q /a.u.) as well as the doublet-quartet energy gap ΔE_{DQ} (eV), and the SOC matrix elements $\langle D_1 | \hat{H}_{\text{SOC}} | Q_1 \rangle$ (cm^{-1}) of all radicals at their respective D_1 geometries.

	E_D	E_Q	ΔE_{DQ}	$\langle D_1 \hat{H}_{\text{SOC}} Q_1 \rangle$
TTM	-4867.34	-4867.29	-1.36	1.23
BN-41-TTM	-4870.77	-4870.71	-1.64	2.61
BN-41-MPTTM	-4642.11	-4642.05	-1.52	3.97
BN-41-metaMPTTM	-4642.16	-4642.11	-1.15	3.57
BN-41-DPTTM	-4413.48	-4413.44	-1.13	2.92
BN-41-metaDPTTM	-4413.53	-4413.48	-1.30	3.75
BN-41-TPTTM	-4184.86	-4184.81	-1.23	6.51

The Cartesian coordinates of TTM.

TTM-D₀

C	0.00007800	0.00001900	-0.00019000
C	0.32994400	1.42659600	-0.00010600
C	-0.26241900	2.33833800	0.89789000
C	1.26248800	1.98599600	-0.89788400
C	0.03811900	3.68953400	0.90724800
C	1.58562400	3.33198100	-0.90681600
C	0.96556600	4.17538300	0.00032200
H	-0.43124300	4.34599900	1.62753200
H	2.29558900	3.71600000	-1.62691200
C	1.07057400	-0.99901400	-0.00011700
C	2.15623600	-0.94233700	0.89806200
C	1.08875300	-2.08596900	-0.89829600
C	3.17597500	-1.87839300	0.90720800
C	2.09274900	-3.03890500	-0.90751300
C	3.13303800	-2.92412600	-0.00014300
H	3.97910200	-1.80057400	1.62759600
H	2.07040200	-3.84544900	-1.62796600
C	-1.40033300	-0.42761900	-0.00023100
C	-1.89413700	-1.39564700	0.89846200
C	-2.35072600	0.09953400	-0.89882300
C	-3.21463900	-1.81077500	0.90782400
C	-3.67796900	-0.29356100	-0.90787700
C	-4.09874800	-1.25132800	0.00004700
H	-3.54884300	-2.54472100	1.62872800
H	-4.36523900	0.12868100	-1.62859700
Cl	-1.34936000	1.78556400	2.12944300
Cl	1.35557400	5.86172500	0.00060300
Cl	1.99664000	1.01253000	-2.12958500
Cl	2.22118000	0.27489400	2.13009200
Cl	-0.12132000	-2.23436600	-2.13014100
Cl	4.39839500	-4.10511900	-0.00009700
Cl	-1.87433100	1.22089400	-2.13142900
Cl	-0.87261400	-2.05941300	2.13119400
Cl	-5.75421100	-1.75660000	0.00022700

TTM-D₁

C	0.00018600	-0.03673000	0.00003600
C	-0.00059100	1.40120500	0.00015500
C	-0.84636600	2.19913700	0.87598800
C	0.84438400	2.20006100	-0.87596700

C	-0.86363900	3.56916900	0.86157600
C	0.86051100	3.57018900	-0.86162300
C	-0.00188200	4.26158500	-0.00010700
H	-1.50730200	4.11222600	1.54122500
H	1.50374300	4.11376400	-1.54126100
C	1.25562700	-0.75255700	0.00445600
C	2.35099400	-0.33691200	0.80510200
C	1.52393700	-1.90057400	-0.78327000
C	3.58462200	-0.96000400	0.82283900
C	2.73647100	-2.56349500	-0.76494700
C	3.76435900	-2.08851900	0.03990900
H	4.37640900	-0.59252900	1.46181400
H	2.89072900	-3.42464900	-1.40169800
C	-1.25502700	-0.75344900	-0.00448400
C	-1.52281300	-1.90074100	0.78423500
C	-2.35004200	-0.33931600	-0.80604200
C	-2.73485200	-2.56468300	0.76598100
C	-3.58318100	-0.96342700	-0.82393900
C	-3.76252700	-2.09125000	-0.03992200
H	-2.88877500	-3.42536100	1.40345000
H	-4.37489100	-0.59720500	-1.46372600
Cl	-1.81982600	1.39679700	2.04508700
Cl	-0.00292400	5.97855600	0.00001300
Cl	1.81861100	1.39838300	-2.04469900
Cl	2.13231400	1.00778300	1.87828700
Cl	0.35058500	-2.47531500	-1.92388300
Cl	5.28768700	-2.91331900	0.05753400
Cl	-2.13182800	1.00460200	-1.88041800
Cl	-0.34935000	-2.47354600	1.92572500
Cl	-5.28532400	-2.91714000	-0.05762500

The Cartesian coordinates of skeleton-engineered radicals at their ground state geometries.

BN-12-TTM-D₀

C	-0.08534900	0.00683300	0.01682100
C	-0.80518200	1.27794200	-0.00950400
C	-0.45110700	2.31670800	-0.89437000
C	-1.87019700	1.57814500	0.86512600
C	-1.09868600	3.53845900	-0.93328200
C	-2.53672300	2.79196900	0.85331000

C	-2.14505400	3.76376300	-0.05308700
H	-0.80034500	4.29377400	-1.64784900
H	-3.33951700	2.97852200	1.55401500
C	-0.82969700	-1.25042500	0.02827000
C	-1.89060800	-1.53089700	-0.85722800
C	-0.49711400	-2.29795000	0.91017700
C	-2.56791900	-2.73872400	-0.86154000
C	-1.15513000	-3.51403700	0.93352800
C	-2.19386600	-3.72173200	0.04006800
H	-3.36474200	-2.91258900	-1.57218500
H	-0.87088400	-4.27813500	1.64444200
C	2.32442400	-0.91526500	-0.92608500
C	3.68735000	-0.87523100	-0.90183600
C	3.65773400	0.79482100	0.85463000
C	4.34563500	-0.01096900	0.00091200
H	4.28303900	-1.48811300	-1.56990500
H	4.14931100	1.45373900	1.55652200
Cl	0.80409200	2.05790000	-2.06364600
Cl	-2.97170300	5.28493000	-0.08304000
Cl	-2.35080500	0.44658400	2.08861500
Cl	-2.35112200	-0.38491500	-2.07424900
Cl	0.74624000	-2.05624500	2.09747800
Cl	-3.03461700	-5.23551200	0.04816300
Cl	1.57907800	1.78823400	2.04100600
Cl	1.56839600	-1.96595000	-2.09154000
Cl	6.07976200	0.02970700	0.02499300
B	1.47380800	-0.03906200	-0.01231500
N	2.29493900	0.78102900	0.84411600

BN-21-TTM-D₀

C	-0.01938000	0.00458300	-0.03215100
C	-1.47391600	-0.04808100	-0.01652200
C	-2.27834600	0.74853300	-0.86093100
C	-2.18106000	-0.90395600	0.85833300
C	-3.66114600	0.70877600	-0.83778300
C	-3.56228100	-0.96832200	0.89124500
C	-4.29395600	-0.15533300	0.04075100
H	-4.23276300	1.32921200	-1.51478600
H	-4.05774500	-1.62725300	1.59141200
C	0.80790300	-1.19610800	-0.01330300
C	0.54168000	-2.28931300	-0.86859100
C	1.92117000	-1.35658700	0.84059800
C	1.30356200	-3.44364800	-0.87373700

C	2.70474500	-2.49779000	0.84423300
C	2.38638600	-3.53690700	-0.01441400
H	1.06613100	-4.24774300	-1.55714200
H	3.53843100	-2.57966300	1.52866800
C	1.55462300	1.60706100	-0.96738800
C	2.24960100	2.77512200	-0.95931900
C	1.07653800	3.55741700	1.02420900
C	2.00341500	3.73971700	0.04755600
H	2.96327200	2.96851000	-1.74647500
H	0.92185000	4.32256100	1.77530000
Cl	-1.56879800	1.77158900	-2.06634200
Cl	-6.02172300	-0.21984100	0.07642600
Cl	-1.34619600	-1.87036000	2.02815300
Cl	-0.72703700	-2.20753500	-2.04587800
Cl	2.32242700	-0.16021300	2.02743900
Cl	3.35356200	-4.97045800	-0.01433100
Cl	-0.81863900	1.88494700	2.32777000
Cl	1.82353900	0.52179700	-2.28065200
Cl	2.94971200	5.19714000	-0.03435400
N	0.60614200	1.28136200	-0.02178500
B	0.32883800	2.25874300	1.02977600

BN-13-TTM-D₀

C	0.09221800	0.03616700	0.01287600
C	-0.03765800	1.49526700	0.03285700
C	-0.85315700	2.16207700	0.96942300
C	0.59901000	2.33561100	-0.90201100
C	-1.02523300	3.53518600	0.98948700
C	0.44674700	3.71277000	-0.91130300
C	-0.36834900	4.30157300	0.04050800
H	-1.64769000	3.99745100	1.74385300
H	0.94641500	4.31068400	-1.66167800
C	1.42801400	-0.56133400	-0.02655500
C	2.45696000	-0.20368700	0.86780700
C	1.76815600	-1.57653500	-0.94341700
C	3.70960900	-0.79537000	0.85870800
C	3.00970600	-2.18634600	-0.98116000
C	3.97465500	-1.78611700	-0.07131000
H	4.45818900	-0.49540700	1.57966200
H	3.22243300	-2.94908300	-1.71811400
C	-1.35814600	-2.13553700	0.83968100
C	-2.52509900	-2.88688600	0.82428700
C	-3.58500400	-2.48640800	0.03998200

H	-2.63302600	-3.78431300	1.42078000
H	-4.31342600	-1.13296100	-1.27969400
Cl	-1.63041000	1.26309300	2.23506600
Cl	-0.56982100	6.02330500	0.04553800
Cl	1.56498200	1.65923400	-2.17531800
Cl	2.17022600	0.96691500	2.11644600
Cl	0.63027600	-2.06125000	-2.16235400
Cl	5.53664500	-2.53719700	-0.09785800
Cl	-2.61617200	0.74961400	-1.85417900
Cl	-0.10607600	-2.72557600	1.89551400
Cl	-5.06466900	-3.35697300	-0.03668600
C	-2.42138000	-0.57322600	-0.75789800
N	-3.50801900	-1.37412900	-0.71199200
B	-1.17954300	-0.86609400	0.03650300

BN-31-TTM-D₀

C	-0.00761000	0.00505100	0.02562100
C	-1.44561900	-0.21465300	0.01947900
C	-2.34166300	0.53087200	-0.77908200
C	-2.04256600	-1.20657300	0.83357400
C	-3.70787500	0.31025100	-0.77614600
C	-3.40337600	-1.44915000	0.84276600
C	-4.22917400	-0.68469800	0.03382400
H	-4.35114800	0.89828700	-1.41676200
H	-3.81402000	-2.20922300	1.49359600
C	0.96445600	-1.07566000	-0.00848600
C	0.80775100	-2.17903600	-0.88182800
C	2.12024300	-1.10937800	0.80502000
C	1.70239100	-3.23159700	-0.92841700
C	3.03277800	-2.14935300	0.76487800
C	2.81309800	-3.20866000	-0.09953800
H	1.54485800	-4.04648600	-1.62199700
H	3.89353000	-2.13709900	1.41985200
C	1.30764500	1.81809400	-0.91370800
C	1.80052600	3.10279300	-0.93130400
C	1.43811300	4.02118200	0.04424100
H	2.45469100	3.37258900	-1.75178600
H	0.15856400	4.36124600	2.03694200
Cl	-1.77429600	1.72527200	-1.89530700
Cl	-5.93236400	-0.97384600	0.04021200
Cl	-1.10079900	-2.12889400	1.95588800
Cl	-0.48477400	-2.23313500	-2.03340000
Cl	2.42900500	0.12098300	1.97993100

Cl	3.94100200	-4.51613900	-0.15061300
Cl	-0.82147400	1.53916400	2.37279800
Cl	1.66070100	0.79931700	-2.25497900
Cl	2.13742800	5.60757200	-0.08050600
N	0.46915400	1.35789400	0.06935300
B	0.50589800	3.65086400	1.14881800
C	0.08666000	2.22320100	1.07113600

BN-14-TTM-D₀

C	-0.09873000	-0.00246700	-0.00067000
C	-0.79835900	-1.28692400	0.02597300
C	-0.44588800	-2.30290800	0.93603200
C	-1.83441800	-1.62233600	-0.86822500
C	-1.06222000	-3.54068200	0.97440500
C	-2.46949600	-2.85342100	-0.85979500
C	-2.07641300	-3.80382400	0.06770700
H	-0.76497000	-4.27888600	1.70705300
H	-3.24836400	-3.06870300	-1.57896300
C	-0.87437700	1.23753700	-0.02622600
C	-1.92788700	1.50997900	0.86900700
C	-0.58419000	2.27310100	-0.93621900
C	-2.63541600	2.70091100	0.86168100
C	-1.27343800	3.47182200	-0.97350800
C	-2.30066800	3.67349100	-0.06572800
H	-3.42511500	2.86899900	1.58162100
H	-1.02151500	4.22680200	-1.70604800
C	2.29689900	1.01198300	0.82898200
C	3.65856200	1.00343100	0.80190900
H	4.27964100	1.65991000	1.39715800
H	4.36975500	-1.40414800	-1.39884700
Cl	0.76496200	-1.99172600	2.13996800
Cl	-2.86356800	-5.34725500	0.09354700
Cl	-2.31744000	-0.51407600	-2.11218000
Cl	-2.34254300	0.37448400	2.11307700
Cl	0.64213600	2.03523400	-2.14117000
Cl	-3.17860900	5.16717100	-0.09006200
Cl	1.70812600	-2.06128800	-1.93747900
Cl	1.58401100	2.16344000	1.93183200
Cl	6.02748800	0.17441400	0.00329300
C	2.35231800	-0.87214600	-0.83238700
B	1.46214700	0.04434400	-0.00146100
N	4.32250000	0.12748600	-0.00044900
C	3.71118300	-0.78502600	-0.80386200

BN-41-TTM-D₀

C	-0.00004400	0.01110800	-0.00019300
C	1.27846700	-0.68410400	-0.01551400
C	2.38141100	-0.29960000	0.78054900
C	1.50277400	-1.80374000	-0.85252100
C	3.59177500	-0.97057500	0.75973400
C	2.70031500	-2.49364600	-0.88054100
C	3.74076200	-2.06990000	-0.06903500
H	4.39992400	-0.64577200	1.40116000
H	2.82476300	-3.33650900	-1.54691200
C	-1.27803700	-0.68506800	0.01527200
C	-1.50129200	-1.80492700	0.85224500
C	-2.38145300	-0.30135300	-0.78051700
C	-2.69829900	-2.49574900	0.88051100
C	-3.59130700	-0.97324300	-0.75944800
C	-3.73926600	-2.07272900	0.06929200
H	-2.82194200	-3.33876300	1.54684100
H	-4.39985600	-0.64900700	-1.40065800
C	-0.62102900	2.15479900	1.01997300
C	-0.68236300	3.50431600	1.07766800
H	-1.18414800	3.93177200	1.93755700
H	1.18133800	3.93287600	-1.93737200
Cl	2.26495900	1.00299800	1.91522100
Cl	5.24499100	-2.92026400	-0.09698800
Cl	0.30032100	-2.33159500	-1.98271400
Cl	-0.29806600	-2.33200100	1.98197700
Cl	-2.26628100	1.00141900	-1.91511600
Cl	-5.24285200	-2.92421800	0.09756800
Cl	1.27086100	1.22318900	-2.32401500
Cl	-1.27160500	1.22197300	2.32389300
Cl	-0.00220600	6.08584300	0.00021700
C	0.61942200	2.15537700	-1.02006800
C	0.67979700	3.50494500	-1.07757700
B	-0.00159300	4.30525000	0.00008300
N	-0.00057000	1.43697800	-0.00010900

BN-23-TTM-D₀

C	0.02054900	-0.01545600	0.05452300
C	-0.30853100	1.41642900	0.02839700
C	-1.17558400	2.00096900	0.97341100
C	0.21465300	2.30148800	-0.93326100

C	-1.50164600	3.34626900	0.96820000
C	-0.08960700	3.65249200	-0.96189500
C	-0.95057300	4.16299000	-0.00550000
H	-2.16072700	3.75072400	1.72455200
H	0.32476700	4.28771300	-1.73315600
C	1.43424400	-0.41513100	0.01949900
C	2.39101200	0.11397200	0.90675800
C	1.93407300	-1.34142200	-0.91805800
C	3.73099400	-0.23497000	0.87209600
C	3.26666900	-1.71268500	-0.97451100
C	4.15714400	-1.15101100	-0.07439500
H	4.42288900	0.18945100	1.58710600
H	3.60426900	-2.41642600	-1.72338800
C	-0.99392000	-2.18116200	0.79572100
C	-2.00122200	-3.16852500	0.77879100
H	-1.89774100	-4.06106000	1.37764200
H	-4.13413900	-1.80326500	-1.27113600
Cl	-1.83064400	1.05757500	2.27458200
Cl	-1.34552900	5.84947500	-0.02621300
Cl	1.21411500	1.71227800	-2.22145600
Cl	1.90814200	1.18433900	2.18233600
Cl	0.90099400	-2.02140500	-2.13477000
Cl	5.82843600	-1.60275500	-0.13384200
Cl	-2.68974300	0.52543900	-1.85132700
Cl	0.31424900	-2.53287200	1.88646700
Cl	-4.37887400	-4.15054000	-0.02945700
C	-1.04394500	-0.98958900	0.07434000
B	-2.31816100	-0.81959500	-0.75590700
C	-3.11783300	-2.98071800	0.02238900
N	-3.28955400	-1.86269500	-0.71836600

BN-32-TTM-D₀

C	0.01160500	-0.01201500	0.03624100
C	-0.09647300	1.44925000	0.02488400
C	0.66446300	2.25541400	-0.84723300
C	-0.98620900	2.14677500	0.86827600
C	0.55153900	3.63472600	-0.88675600
C	-1.12362600	3.52352800	0.84394700
C	-0.34903100	4.25825600	-0.03913300
H	1.14555800	4.20874100	-1.58507600
H	-1.81061900	4.01363300	1.52062300
C	-1.19714700	-0.83495200	-0.01095600
C	-2.23371700	-0.61114700	-0.93973000

C	-1.40761600	-1.90320900	0.88514200
C	-3.38762900	-1.37441900	-0.97564100
C	-2.54926400	-2.68510900	0.86794600
C	-3.53463900	-2.40937000	-0.06623900
H	-4.14882100	-1.17497200	-1.71785700
H	-2.67344100	-3.48403000	1.58649400
C	1.67410600	-1.68766100	-0.79163300
C	2.95947800	-2.25978800	-0.82508800
H	3.14451500	-3.05342400	-1.54135500
H	4.39790000	-0.25484000	1.79528400
Cl	1.74201100	1.54196700	-2.00127200
Cl	-0.50647400	5.98046100	-0.08074800
Cl	-1.90139600	1.30524700	2.07507800
Cl	-2.06703800	0.59206700	-2.17492200
Cl	-0.26066600	-2.24055400	2.14020800
Cl	-4.97052400	-3.37395400	-0.09898000
Cl	1.85611000	0.85730100	2.19768200
Cl	0.58733400	-2.23443700	-2.02549700
Cl	5.52171300	-2.51628000	-0.07597100
C	1.30965300	-0.65486300	0.06939500
C	3.94596400	-1.79519900	-0.00279400
N	2.30805300	-0.21748700	0.92864600
B	3.65232300	-0.69498000	0.98656000

BN-24-TTM-D₀

C	0.01093700	-0.00856700	0.04567000
C	-1.32703700	-0.62175600	0.01301800
C	-1.73056400	-1.57469500	0.96868300
C	-2.29358600	-0.29206200	-0.95402600
C	-2.98679000	-2.15575500	0.96900500
C	-3.55889800	-0.85521900	-0.97920100
C	-3.89334600	-1.78601700	-0.01085600
H	-3.25553900	-2.87379500	1.73191800
H	-4.26082700	-0.58329100	-1.75586900
C	0.09624800	1.46181300	0.02599800
C	-0.61938200	2.27347600	0.92587600
C	0.87645100	2.15673900	-0.91993400
C	-0.57864400	3.65773000	0.89378400
C	0.93784400	3.53895100	-0.97561300
C	0.20356900	4.27943000	-0.06431400
H	-1.13549900	4.23590400	1.61880800
H	1.53904600	4.02665900	-1.73104800
C	2.36479900	-0.49050800	0.72967400

C	3.52860000	-1.22726900	0.69864700
H	4.40972900	-0.94661000	1.25333400
H	2.79379600	-3.79929200	-1.26395900
Cl	-0.67500000	-2.02754800	2.26900700
Cl	-5.47094100	-2.50121400	-0.02469200
Cl	-1.90634000	0.78595700	-2.25471200
Cl	-1.53179500	1.56225000	2.21652300
Cl	1.76592900	1.30429300	-2.14002800
Cl	0.26758400	6.00931300	-0.12270800
Cl	-0.02683400	-2.85713800	-1.74271600
Cl	2.46081100	0.88455100	1.79781100
Cl	5.10440100	-3.18558900	-0.01318000
C	1.17268300	-0.84384200	0.05409300
C	2.57399600	-2.88780500	-0.72359700
B	1.26424700	-2.16003900	-0.72244100
N	3.59056100	-2.36859200	-0.02466100

BN-42-TTM-D₀

C	0.01361200	-0.02989100	0.01995000
C	0.02903200	1.43523100	0.02877800
C	0.84317400	2.18638700	-0.84550700
C	-0.78710400	2.19550500	0.89260900
C	0.84058700	3.57052400	-0.87263800
C	-0.81451500	3.57903900	0.88073600
C	0.00354800	4.25731300	-0.00840600
H	1.46982900	4.10113800	-1.57450700
H	-1.45067800	4.11659500	1.57102600
C	-1.26410200	-0.74278900	-0.01520000
C	-2.29983500	-0.40549400	-0.91067500
C	-1.54919400	-1.80914900	0.86255000
C	-3.51905000	-1.05971900	-0.93084100
C	-2.75726200	-2.48418500	0.86012500
C	-3.73705400	-2.09838600	-0.04015400
H	-4.27728600	-0.77508000	-1.64781700
H	-2.93456500	-3.28633000	1.56382800
C	1.53167700	-1.84075700	-0.89438700
C	2.72238500	-2.51814600	-0.95802600
H	2.81450100	-3.28738100	-1.71795700
H	4.12680000	-0.63924300	1.70783600
Cl	1.85178700	1.39855000	-2.01373900
Cl	-0.01605700	5.98683400	-0.03520800
Cl	-1.74672900	1.41874800	2.10926600
Cl	-2.05699600	0.80484400	-2.12645200

Cl	-0.40701600	-2.28646100	2.07784800
Cl	-5.25501800	-2.92838100	-0.05487300
Cl	1.93540400	0.65453500	2.15087300
Cl	0.33071000	-2.22229700	-2.09666800
Cl	5.44088700	-2.88168200	-0.00631900
C	1.24539700	-0.78263800	0.01352100
N	2.26847300	-0.46600400	0.87908400
C	3.48753400	-1.02096700	0.92218600
B	3.82611100	-2.12373600	-0.03282200

BN-25-TTM-D₀

C	0.02367200	0.00337800	-0.01988300
C	1.47161000	-0.22904300	-0.03062600
C	2.08711400	-1.09289900	-0.95851300
C	2.34593700	0.38550200	0.88706400
C	3.44911300	-1.33893100	-0.97439000
C	3.71282400	0.16348500	0.89245900
C	4.25278600	-0.70346900	-0.04232500
H	3.87496400	-2.00096000	-1.71624700
H	4.33922700	0.64485200	1.63129000
C	-0.48697200	1.37900700	0.00120800
C	-0.05938100	2.35568700	-0.91991500
C	-1.44032100	1.81977000	0.94227900
C	-0.52693500	3.65944900	-0.91301600
C	-1.92960200	3.11474200	0.96994600
C	-1.46440500	4.02722600	0.03720000
H	-0.17645600	4.36743800	-1.65195700
H	-2.64703400	3.40900300	1.72416600
C	-2.01595600	-1.17825400	-0.76398000
H	-3.71293600	-2.14792700	-1.35097300
H	-1.69516500	-4.33601900	1.52547500
Cl	1.15931600	-1.84061300	-2.22060700
Cl	5.95994000	-0.99661000	-0.04813800
Cl	1.72881500	1.40107800	2.14892500
Cl	1.03363700	1.93754600	-2.19958100
Cl	-1.99278800	0.76588200	2.20382400
Cl	-2.06415700	5.65200900	0.06079600
Cl	0.67525900	-2.49130500	2.06504800
Cl	-2.43381900	0.00492800	-1.95210900
Cl	-4.08061900	-4.41856700	-0.07691700
C	-0.88156900	-1.13634100	0.01116500
C	-1.73055600	-3.44773500	0.90718500
B	-0.68882600	-2.35711100	0.92852700

N	-2.91976000	-2.19547200	-0.72824200
C	-2.78320400	-3.28597800	0.07617500

BN-52-TTM-D₀

C	0.02256400	-0.03211500	0.01467800
C	-0.35722000	1.38187700	-0.00277000
C	-1.31619700	1.92344300	0.87963300
C	0.21928500	2.30152700	-0.90530100
C	-1.67170300	3.26154300	0.87309400
C	-0.11381000	3.64440900	-0.92686900
C	-1.06181900	4.11425200	-0.03216400
H	-2.39925200	3.63291300	1.58224600
H	0.34709600	4.30741800	-1.64665200
C	1.43139200	-0.42104400	0.01408200
C	2.37660700	0.16283600	0.88316800
C	1.93820000	-1.40785700	-0.85621100
C	3.71273500	-0.19678700	0.88817600
C	3.26811900	-1.78893500	-0.86863300
C	4.14774300	-1.17434700	0.00782500
H	4.39731100	0.26556900	1.58643900
H	3.61275000	-2.54061500	-1.56591700
C	-1.01263000	-2.13193900	0.96405600
H	-2.11222800	-4.06201000	1.81124400
H	-3.87447800	-1.64334500	-1.58538700
Cl	-2.04403000	0.94176000	2.10470100
Cl	-1.49123600	5.78924700	-0.04760400
Cl	1.32804100	1.76834400	-2.12597700
Cl	1.88523600	1.31093500	2.08290600
Cl	0.91643200	-2.14361000	-2.04721100
Cl	5.81456900	-1.63567100	0.00387600
Cl	-1.99423100	0.04991700	-2.15974800
Cl	0.21513000	-2.18962100	2.19818300
Cl	-4.64801900	-3.88954200	-0.06572200
C	-0.99785600	-1.07804000	0.06348600
C	-3.13177000	-1.85515100	-0.82682800
C	-3.21548400	-2.90131600	0.04114100
B	-2.11383700	-3.16518400	1.02951200
N	-2.07472800	-0.99686500	-0.80439700

BN-26-TTM-D₀

C	0.00944600	-0.04542400	0.07887000
C	-1.40077800	-0.45761000	0.00714700

C	-1.96750700	-1.32562200	0.96052000
C	-2.27857800	0.00170800	-0.99064300
C	-3.29674200	-1.70910100	0.93152700
C	-3.61379400	-0.36203300	-1.04459700
C	-4.11070100	-1.21802800	-0.07647200
H	-3.69171800	-2.36919800	1.69188800
H	-4.24624500	0.00217700	-1.84290800
C	0.31321800	1.39542600	0.05007600
C	-0.32393400	2.32083100	0.89894800
C	1.22470200	1.95273200	-0.87073500
C	-0.10193400	3.68623600	0.83238700
C	1.46928100	3.31306700	-0.95688700
C	0.79578300	4.17154100	-0.10363700
H	-0.61004700	4.35438300	1.51471700
H	2.16444700	3.69472900	-1.69251100
H	4.13739100	-1.31534400	1.33752300
H	2.30014500	-4.09241400	-1.35702300
Cl	-1.02288800	-1.92243300	2.28850800
Cl	-5.77718300	-1.68509300	-0.12682400
Cl	-1.69320900	0.98762300	-2.28960800
Cl	-1.36906400	1.77239700	2.16753200
Cl	2.06161600	0.95256600	-2.01267800
Cl	1.08685400	5.87477800	-0.20383900
Cl	-0.42664800	-2.84510500	-1.69042800
Cl	2.33892000	0.43430000	1.94027900
Cl	4.81483300	-3.64881200	-0.06796100
C	1.01311000	-1.04466100	0.10907900
C	2.22145100	-3.18571800	-0.76677100
C	3.31863600	-2.76027100	-0.05855700
N	2.19902300	-0.83737300	0.77994600
B	0.97746400	-2.35454100	-0.70863500
C	3.30177900	-1.61369800	0.72427500

BN-34-TTM-D₀

C	0.01747700	-0.01619300	0.02082800
C	1.40655200	-0.48017200	0.00780900
C	1.86159100	-1.46303000	-0.89403700
C	2.38046900	0.02546100	0.89236600
C	3.16973000	-1.91455400	-0.91820700
C	3.69610500	-0.40483200	0.88737900
C	4.07908600	-1.37674200	-0.02227100
H	3.47533000	-2.65961900	-1.64034100
H	4.40335700	-0.00010700	1.59871700

C	-0.27403300	1.41910600	0.00808000
C	0.33454400	2.30377600	-0.90643000
C	-1.17965600	2.01455200	0.91010100
C	0.07260500	3.66277300	-0.92706700
C	-1.46352200	3.36960300	0.90781200
C	-0.82999700	4.18488000	-0.01519100
H	0.55262400	4.29778000	-1.65946000
H	-2.15366800	3.78157200	1.63170500
H	-4.04525200	-1.66743200	-1.55880200
H	-2.34270600	-3.98108700	1.72611300
Cl	0.80469000	-2.09755700	-2.11189000
Cl	5.71989300	-1.92716900	-0.04032100
Cl	1.94841300	1.16463600	2.12403400
Cl	1.39058900	1.70885500	-2.14479100
Cl	-1.92591400	1.07622200	2.16031400
Cl	-1.17053100	5.88162300	-0.02919200
Cl	0.11266400	-2.25208400	2.15612400
Cl	-2.20600500	0.31427000	-2.10466100
Cl	-4.66280400	-3.78828900	-0.04859200
C	-1.07334900	-0.99650500	0.05172000
C	-3.23308200	-1.75563400	-0.85065700
C	-2.18552900	-0.88790900	-0.85086400
C	-1.10938300	-2.06718600	0.93380200
N	-3.26779500	-2.78971300	0.03384800
B	-2.24393100	-3.06322100	0.98333500

BN-43-TTM-D₀

C	0.00599000	-0.01113000	0.01919900
C	-0.16450800	1.44261300	0.00237000
C	-1.01806900	2.11368200	0.90350100
C	0.50822500	2.27362600	-0.91766100
C	-1.19254500	3.48681400	0.89641100
C	0.35671400	3.64954400	-0.94344600
C	-0.49832000	4.24597600	-0.03156100
H	-1.84457300	3.95562500	1.62112500
H	0.88419500	4.24109100	-1.67962200
C	1.35037900	-0.59077300	0.00083500
C	2.37119900	-0.15361500	0.87108200
C	1.72058200	-1.62495100	-0.88377500
C	3.64732400	-0.68949300	0.86763300
C	2.98693800	-2.18380400	-0.90435700
C	3.94390100	-1.70707100	-0.02401600
H	4.38984000	-0.32999000	1.56724100

H	3.22473800	-2.96494400	-1.61379200
H	-2.40645600	-3.57779200	1.80049700
H	-4.00444800	-1.28207900	-1.55670800
Cl	-1.83519000	1.24378000	2.16068600
Cl	-0.70282700	5.96483000	-0.05175300
Cl	1.51156900	1.58971300	-2.15551000
Cl	2.04601600	1.03969100	2.08571000
Cl	0.61617800	-2.20067500	-2.09140800
Cl	5.53357800	-2.39213400	-0.03878100
Cl	-2.17182100	0.45456000	-2.10635200
Cl	-0.08472200	-2.15298800	2.20599800
Cl	-4.98221100	-3.54050700	-0.06755200
C	-1.17008000	-0.88157000	0.04885300
C	-2.38438400	-2.80997700	1.03674200
C	-1.31826100	-1.96409000	0.99202100
C	-2.21283500	-0.71626500	-0.84367400
B	-3.49173600	-2.58864400	0.05388300
N	-3.31397400	-1.49748100	-0.84953300

BN-35-TTM-D₀

C	0.02501400	-0.01569000	0.04294700
C	1.44872400	-0.35393400	0.00404600
C	1.97674200	-1.31580800	-0.88076800
C	2.38941200	0.25853200	0.85791200
C	3.31871700	-1.65313600	-0.91465100
C	3.73739900	-0.05511700	0.84133600
C	4.19088500	-1.01512000	-0.04825200
H	3.67710200	-2.38819700	-1.62264900
H	4.41663800	0.42925100	1.52984100
C	-0.40108400	1.38402900	0.01377000
C	0.10211800	2.30522200	-0.92926900
C	-1.34884300	1.90780100	0.91847300
C	-0.29148900	3.63175000	-0.97178300
C	-1.76394600	3.22828200	0.89387900
C	-1.22706700	4.08257400	-0.05516800
H	0.11338500	4.29501400	-1.72429800
H	-2.47942500	3.58627600	1.62195100
H	-3.71742000	-2.00243100	-1.46928100
H	-1.90024900	-4.15718700	1.89812100
Cl	0.96868100	-2.07193600	-2.07192500
Cl	5.87269300	-1.42255700	-0.07875300
Cl	1.88023400	1.39108600	2.06628700
Cl	1.19327000	1.79082600	-2.17438000

Cl	-1.98003800	0.92773600	2.19895300
Cl	-1.73263900	5.73716200	-0.09613000
Cl	0.31641200	-2.11721000	2.25718100
Cl	-2.22420600	0.01506200	-2.08160400
Cl	-4.34668300	-4.16263500	-0.12078700
C	-0.97603800	-1.09319800	0.11090900
C	-2.04320700	-1.10762900	-0.79118000
C	-0.92890600	-2.15220500	1.04304900
N	-2.98271700	-2.06822800	-0.77256200
B	-1.92642000	-3.26766900	1.11022900
C	-2.99346400	-3.10882800	0.08854900

The Cartesian coordinates of skeleton-engineered radicals at their lowest excited state geometries.

BN-21-TTM-D₁

C	-0.05820500	0.00836900	-0.01990600
C	1.82169400	1.22475800	-0.93337200
C	1.66578100	3.40937300	0.80517900
C	2.90435600	2.18607200	-0.83295100
C	2.81323300	3.26403600	-0.00640800
H	1.59377000	4.26133600	1.47174200
H	3.76693600	2.02536900	-1.46571100
C	0.57170200	-1.29717200	-0.00882000
C	1.65641200	-1.62548200	0.83774300
C	0.13841800	-2.36214500	-0.83379300
C	2.25773500	-2.87035400	0.86613800
C	0.70017300	-3.62757000	-0.80473900
C	1.76655200	-3.87188800	0.04329200
H	3.07387400	-3.06477100	1.54916800
H	0.32509600	-4.40203000	-1.46041300
C	-1.49077300	0.18864600	0.00531400
C	-2.33350900	-0.54996300	0.87313700
C	-2.17951200	1.10457500	-0.82529500
C	-3.70894200	-0.40970200	0.90118000
C	-3.55016000	1.28882900	-0.79538000
C	-4.31163000	0.51848800	0.06745400
H	-4.29827600	-0.99634400	1.59310900
H	-4.01724800	2.00024800	-1.46322800
Cl	-0.66759500	2.39238000	1.99989800
Cl	4.09745300	4.41797100	0.07489800

Cl	1.90060400	0.17722200	-2.26728800
Cl	2.24325300	-0.47298100	2.00323300
Cl	-1.11443200	-2.10552800	-2.00527700
Cl	2.49440700	-5.44413200	0.07956000
Cl	-1.31929200	2.02086200	-2.03058100
Cl	-1.65272500	-1.63317700	2.04428300
Cl	-6.03260600	0.71804200	0.10501300
N	0.76683900	1.14554100	-0.06342600
B	0.61477900	2.29659700	0.82461900

BN-14-TTM-D₁

C	0.10323800	0.04803400	0.00200900
C	1.29804000	-0.76913900	0.00627000
C	1.40675000	-1.93144400	-0.79750800
C	2.45191300	-0.52865800	0.79057800
C	2.51163700	-2.76239600	-0.84120900
C	3.58489900	-1.32334500	0.76101000
C	3.60835600	-2.43991300	-0.05978100
H	2.52581400	-3.62824700	-1.48961500
H	4.42949000	-1.08612200	1.39457100
C	0.20247400	1.49202500	-0.00308400
C	1.10554800	2.24842300	-0.78866800
C	-0.64291400	2.29777200	0.79999600
C	1.18331700	3.63003300	-0.76000400
C	-0.61057500	3.67999900	0.84291800
C	0.32174100	4.34069100	0.06108600
H	1.89221200	4.14603400	-1.39418000
H	-1.28158900	4.22781300	1.49101700
C	-2.53909900	-0.05983200	-0.74206000
C	-3.73743200	-0.70458800	-0.71220000
H	-4.61739400	-0.38489000	-1.25370200
H	-3.18030200	-3.37397700	1.25505100
Cl	0.08648200	-2.34861700	-1.86475500
Cl	5.02277400	-3.44835900	-0.10249000
Cl	2.46382800	0.77988500	1.93587300
Cl	2.13869000	1.44656900	-1.93465400
Cl	-1.78974000	1.52071300	1.86555100
Cl	0.40662000	6.07568700	0.10322500
Cl	-0.50991800	-2.77111400	1.74728500
Cl	-2.47545600	1.31844900	-1.75298400
Cl	-5.39913000	-2.60150200	-0.00133300
C	-1.62679600	-1.95695600	0.73939400
B	-1.23369200	-0.59954200	-0.00105600

N	-3.87078600	-1.86595700	0.00068300
C	-2.88023000	-2.48742100	0.71295100

BN-41-TTM-D₁

C	-0.01750300	-0.00019600	-0.00012400
C	0.64724700	1.26318800	-0.00998900
C	0.20225100	2.44002400	0.66158100
C	1.86551100	1.46661300	-0.77356500
C	0.89222400	3.62954800	0.62001600
C	2.59352600	2.64537100	-0.78041900
C	2.09858900	3.73450000	-0.09336300
H	0.52148100	4.47913200	1.17927900
H	3.50379600	2.71633600	-1.36092400
C	0.66349300	-1.25489700	0.00992800
C	1.88395200	-1.44267900	0.77403000
C	0.23400700	-2.43731000	-0.66194100
C	2.62717800	-2.61188800	0.78096500
C	0.93931300	-3.61781000	-0.62027900
C	2.14672700	-3.70719700	0.09346200
H	3.53800900	-2.67111800	1.36188700
H	0.57980200	-4.47209800	-1.17971900
C	-2.15920400	-0.59616900	1.03406300
C	-3.51071600	-0.67504300	1.09579400
H	-3.93469600	-1.16543800	1.96386000
H	-3.94937600	1.11502000	-1.96385000
Cl	-1.19020000	2.40589400	1.69167800
Cl	2.94527000	5.23594800	-0.10046000
Cl	2.42252000	0.20529900	-1.79914300
Cl	2.42409800	-0.17456100	1.80021800
Cl	-1.15836900	-2.42098200	-1.69256500
Cl	3.01300000	-5.19741400	0.10034600
Cl	-1.21956700	1.20356800	-2.33654600
Cl	-1.20391100	-1.21945100	2.33617600
Cl	-6.09818200	-0.03855300	0.00031400
C	-2.16669800	0.56821300	-1.03431900
C	-3.51910900	0.63002300	-1.09584500
B	-4.31246500	-0.02747100	0.00007400
N	-1.44437400	-0.00941900	-0.00016500

BN-23-TTM-D₁

C	0.05512000	-0.02172100	0.06229200
C	1.50328800	-0.08802400	0.02928500

C	2.30765000	0.65538900	0.92955400
C	2.22022100	-0.87329400	-0.90749300
C	3.68748800	0.63195900	0.90335700
C	3.60168500	-0.90354100	-0.95788800
C	4.32804200	-0.14848900	-0.04994200
H	4.25632400	1.19845300	1.62827200
H	4.10366800	-1.49446700	-1.71215800
C	-0.73590300	-1.24281300	-0.03424900
C	-0.47922100	-2.38322600	0.76221900
C	-1.85117000	-1.35083000	-0.89861600
C	-1.27321400	-3.51428700	0.73009100
C	-2.65659700	-2.47311700	-0.95086600
C	-2.36441700	-3.54844500	-0.12569000
H	-1.05393200	-4.35004500	1.38089900
H	-3.48636400	-2.51606900	-1.64353300
C	-1.79794800	1.44007700	0.94985600
C	-2.56099000	2.58467200	0.87279700
H	-3.44274900	2.69633300	1.48910000
H	-0.79862500	4.43534600	-1.22111000
Cl	1.57976900	1.56636200	2.21047500
Cl	6.05534800	-0.17876200	-0.10413300
Cl	1.39390100	-1.76721700	-2.13981100
Cl	0.80583900	-2.38343000	1.92487500
Cl	-2.19565300	-0.11055400	-2.06132000
Cl	-3.36945200	-4.95506200	-0.16964600
Cl	1.22626100	2.54060600	-1.74799300
Cl	-2.20584700	0.31887000	2.21342700
Cl	-3.20711200	5.00524900	-0.16773000
C	-0.59892300	1.24484100	0.15814000
C	-2.19375800	3.63584400	0.03422300
B	-0.18312700	2.45684300	-0.68218200
N	-1.03181600	3.60903200	-0.69162700

BN-32-TTM-D₁

C	0.01818000	0.01944000	0.03568000
C	1.43343700	-0.33077500	0.01504600
C	1.96050400	-1.32125500	-0.83981500
C	2.38890900	0.27475500	0.86250500
C	3.29229300	-1.69684400	-0.85800200
C	3.73232600	-0.05722700	0.85134700
C	4.17476700	-1.04940800	-0.00941800
H	3.63720500	-2.45831100	-1.54469900
H	4.41864000	0.43462100	1.52782800

C	-0.42011400	1.39306300	-0.00036000
C	0.21186200	2.40128400	-0.77622900
C	-1.53549000	1.86311500	0.73821100
C	-0.18210200	3.72656100	-0.76915400
C	-1.96848500	3.17573100	0.74540000
C	-1.27159300	4.11019800	-0.00208300
H	0.33798300	4.44666400	-1.38694600
H	-2.82030100	3.46589100	1.34591300
C	-2.07068600	-1.11892700	-0.88428700
C	-3.06640200	-2.08710000	-0.85682300
H	-3.87884100	-2.01189500	-1.57205900
H	-1.52893600	-4.14324700	1.67682500
Cl	0.92030400	-2.08346200	-2.00712900
Cl	5.85317700	-1.48502800	-0.02361700
Cl	1.89035600	1.44306600	2.04409700
Cl	1.48145000	1.99543300	-1.88785500
Cl	-2.40980800	0.75909900	1.75556500
Cl	-1.77629800	5.76800100	0.00565000
Cl	0.26214700	-2.04355200	2.17288800
Cl	-2.14349400	0.05896300	-2.11955400
Cl	-4.18705300	-4.37261500	0.01305200
C	-0.94504800	-1.04893700	0.04098100
C	-2.96851600	-3.15550600	0.01088700
N	-0.87479700	-2.10283100	0.89301600
B	-1.77769800	-3.25625600	0.93521500

BN-25-TTM-D₁

C	0.06794200	-0.08116800	0.01853200
C	-1.58626900	1.62641100	0.84947800
C	-0.74754800	3.73589200	-0.89263800
C	-1.82208800	3.83546400	-0.07609900
H	-3.02915200	2.97178200	1.33294200
H	-0.51035700	4.57609600	-1.53306900
C	1.49870300	-0.21882400	0.04037300
C	2.31622500	0.67488700	0.78289200
C	2.24314400	-1.18518500	-0.68664900
C	3.69783800	0.66977400	0.78755000
C	3.62330900	-1.24488000	-0.67134500
C	4.34870300	-0.31483900	0.06410400
H	4.25100700	1.39089700	1.37438500
H	4.13456800	-1.99030200	-1.26638300
C	-0.81378500	-1.22524100	-0.01025000
C	-0.63374200	-2.40113300	0.76089900

C	-1.98047600	-1.25012000	-0.81268400
C	-1.49409500	-3.48323900	0.71156600
C	-2.87808900	-2.29969700	-0.86342100
C	-2.61556600	-3.42765100	-0.10278500
H	-1.30672100	-4.35007800	1.33160800
H	-3.74462600	-2.25185900	-1.50944600
Cl	-2.24789700	0.58188200	2.02602100
Cl	-2.82525600	5.23441500	0.03558400
Cl	1.31793400	2.17541800	-2.05299200
Cl	1.53108600	1.84789300	1.80111200
Cl	1.44123600	-2.28887200	-1.75848000
Cl	6.08107200	-0.38759400	0.06940200
Cl	-2.29519600	0.10515700	-1.85810500
Cl	0.66447200	-2.50092400	1.90923200
Cl	-3.70457000	-4.77750200	-0.16111700
C	-0.48764200	1.25401500	0.01300100
B	-0.00709400	2.42221700	-0.92018500
N	-2.22108700	2.81824900	0.74494100

BN-52-TTM-D₁

C	0.01258300	-0.01699700	-0.00498400
C	-0.04719000	1.44282200	-0.02518600
C	-0.83673600	2.18620700	0.87680500
C	0.68713500	2.22647700	-0.94045200
C	-0.90389800	3.56917000	0.87884900
C	0.66441400	3.61083600	-0.94992800
C	-0.13967000	4.27345400	-0.03673500
H	-1.51971300	4.08588800	1.60279400
H	1.24699200	4.16061000	-1.67715200
C	1.29052200	-0.69651500	0.01556700
C	2.40860800	-0.25590500	0.76933200
C	1.54289400	-1.86958000	-0.74164500
C	3.64452300	-0.87368800	0.73266400
C	2.75969400	-2.52944500	-0.77245900
C	3.81485100	-2.01073600	-0.04420700
H	4.45767100	-0.49127500	1.33535700
H	2.88429300	-3.41602000	-1.37972200
C	-1.37152000	-1.96856300	0.87350000
H	-2.73489400	-3.79484700	1.55286600
H	-4.29462500	-0.59120100	-1.24973300
Cl	-1.73971900	1.36429200	2.11566000
Cl	-0.19147500	6.00726000	-0.04141700
Cl	1.62393000	1.45638300	-2.18249600

Cl	2.25010500	1.05885200	1.89082100
Cl	0.29209000	-2.52673700	-1.74962600
Cl	5.35893000	-2.79650400	-0.08654400
Cl	-2.18344800	0.70347300	-1.90228600
Cl	-0.18192200	-2.29273500	2.04716000
Cl	-5.30361100	-2.99149600	-0.09442100
C	-1.17862000	-0.77641000	0.06277800
C	-3.54381800	-1.09819500	-0.65898100
C	-3.74470500	-2.25061500	0.00056500
B	-2.61258300	-2.83580000	0.86348500
N	-2.29345000	-0.46506400	-0.66588700

BN-34-TTM-D₁

C	0.03258100	0.00681200	0.02025800
C	-0.72609100	1.25304200	0.03770100
C	-0.41892300	2.34480700	-0.80845400
C	-1.85866400	1.46632100	0.85784500
C	-1.15307100	3.51860000	-0.85335900
C	-2.62759400	2.61623400	0.82041400
C	-2.26688500	3.63910400	-0.04211400
H	-0.87096300	4.31201500	-1.53234200
H	-3.47775800	2.72264900	1.48094600
C	-0.72196700	-1.24699400	-0.03501300
C	-1.72874700	-1.49082600	-0.99205300
C	-0.53107000	-2.29721400	0.88825200
C	-2.49115400	-2.64701100	-1.02508000
C	-1.26033000	-3.47399800	0.87331000
C	-2.24606600	-3.63466300	-0.08619100
H	-3.24556100	-2.78140200	-1.78870800
H	-1.07756700	-4.23980600	1.61516500
H	4.21082800	-1.70067600	-1.11513400
H	4.39646400	1.90584400	1.32402300
Cl	0.90622500	2.23775800	-1.92563500
Cl	-3.21566200	5.09059700	-0.09559900
Cl	-2.29331300	0.30323700	2.07142800
Cl	-2.00355000	-0.35149600	-2.27350200
Cl	0.63043700	-2.13110600	2.17190200
Cl	-3.18387200	-5.09464800	-0.11354100
Cl	1.46308500	2.10632600	1.84073500
Cl	1.64802400	-2.19859000	-1.54482700
Cl	6.09565100	-0.03526400	-0.13651900
C	1.43772000	0.02047700	0.07929800
C	3.68223300	-0.92732900	-0.57054700

C	2.28036200	-0.94394700	-0.55533800
C	2.23335200	1.01584300	0.76163600
N	4.39850800	0.02354200	0.01603800
B	3.73229300	1.10903500	0.75498100

BN-43-TTM-D₁

C	-0.03378000	0.03976200	-0.02358200
C	0.67273300	1.29048000	-0.01539100
C	1.88517000	1.50563100	-0.72478900
C	0.25685500	2.43353200	0.72629800
C	2.58837400	2.69403400	-0.74278100
C	0.92230000	3.64516100	0.70421400
C	2.08725600	3.77512900	-0.03621800
H	3.49652400	2.78107400	-1.32440500
H	0.55078800	4.47226400	1.29482500
C	-1.48194000	-0.02529400	0.01573800
C	-2.32319400	0.76805500	-0.80348600
C	-2.18328900	-0.93802100	0.83421500
C	-3.70235500	0.66397100	-0.80356200
C	-3.55801900	-1.09052800	0.83818800
C	-4.31396300	-0.27368200	0.01483400
H	-4.29109000	1.28767900	-1.46315700
H	-4.02868600	-1.80748700	1.49760100
H	0.90798600	-4.18076200	-1.76114700
H	3.30957400	-2.59187100	1.54263200
Cl	2.53232700	0.21575900	-1.69641700
Cl	2.93216600	5.28979800	-0.06017900
Cl	-1.09106800	2.33659700	1.81878100
Cl	-1.63623300	1.87795700	-1.94653700
Cl	-1.29381000	-1.89104600	1.98997100
Cl	-6.04299100	-0.42221800	0.00804500
Cl	2.02607600	-0.39122900	2.19089400
Cl	-0.73290600	-2.00865300	-2.21189500
Cl	3.39318700	-5.01972500	-0.03586000
C	0.69412000	-1.22120700	-0.03570200
C	1.15664000	-3.44400500	-1.00598400
C	0.45149600	-2.27319000	-0.98180500
C	1.72872500	-1.49468500	0.93832300
B	2.32444600	-3.62704100	-0.04707600
N	2.55360100	-2.56280400	0.87033200

The Cartesian coordinates of periphery-engineered radicals at their ground state geometries.

BN-41-MPTTM-D₀

C	-0.65988000	-0.00007500	-0.00001600
C	-1.35665600	1.27818700	-0.01158400
C	-0.97359400	2.36184800	-0.83411800
C	-2.47506000	1.52220700	0.82077900
C	-1.64397200	3.57291800	-0.84017700
C	-3.16481400	2.72033300	0.82253500
C	-2.74153200	3.74153900	-0.01302800
H	-1.32018400	4.36576700	-1.50092400
H	-4.00678700	2.86015100	1.48697100
C	-1.35850800	-1.27728700	0.01140900
C	-2.47708200	-1.51962700	-0.82122500
C	-0.97728900	-2.36149100	0.83406800
C	-3.16874700	-2.71663700	-0.82300200
C	-1.64961600	-3.57150200	0.84010800
C	-2.74729600	-3.73843300	0.01279100
H	-4.01074100	-2.85523300	-1.48766800
H	-1.32719000	-4.36478700	1.50099800
C	1.48627700	-0.65463500	-0.99576900
C	2.83382600	-0.71763800	-1.04423500
H	3.23995000	-1.24317100	-1.90188000
H	3.24057200	1.23951000	1.90271300
Cl	0.32623900	2.21683600	-1.96866300
Cl	-3.59124700	5.24741300	-0.01793200
Cl	-3.00228100	0.34525800	1.97834000
Cl	-3.00194000	-0.34205600	-1.97923200
Cl	0.32274600	-2.21863400	1.96866500
Cl	-3.59946200	-5.24292800	0.01765400
Cl	0.55296100	1.33489000	2.28958100
Cl	0.55233000	-1.33768700	-2.28855100
C	1.48660500	0.65203200	0.99646600
C	2.83417500	0.71456500	1.04483900
B	3.67461700	-0.00152900	0.00014900
N	0.76207300	-0.00102700	0.00029100
C	5.23665300	-0.00175100	0.00008600
C	5.96867400	-0.90941900	-0.78097900
C	5.96893600	0.90576800	0.78107700
C	7.35716800	-0.91737800	-0.78052700
H	5.44151100	-1.63374300	-1.39527200
C	7.35743200	0.91345900	0.78047600

H	5.44196900	1.63020400	1.39540600
C	8.05567700	-0.00202900	-0.00006000
H	7.89730000	-1.63533400	-1.38957000
H	7.89776900	1.63131300	1.38945900
H	9.14108700	-0.00213600	-0.00011700

BN-41-metaMPTTM-D₀

C	0.66187500	-0.01370100	0.00401400
C	-0.79112700	-0.02448300	-0.00026000
C	-1.56983200	-0.90169100	0.78922800
C	-1.54045400	0.85423300	-0.81966500
C	-2.95148400	-0.89259700	0.77618900
C	-2.92026700	0.87506800	-0.83164500
C	-3.65616100	0.00083100	-0.03026400
H	-3.48049100	-1.60107900	1.40126900
H	-3.42470200	1.58636700	-1.47354100
C	1.44533600	1.21320600	0.02220200
C	1.10732400	2.29453200	0.87138600
C	2.59066900	1.41759200	-0.78026000
C	1.82261100	3.47709800	0.90462700
C	3.32662200	2.58965000	-0.75467100
C	2.93212600	3.61638900	0.08633000
H	1.52888200	4.26905900	1.58020700
H	4.18618500	2.70149100	-1.40172500
C	2.24854900	-1.59788900	1.00255100
C	2.95897300	-2.74790700	1.04611400
H	3.60876000	-2.88589500	1.90205600
H	1.52341000	-3.99848100	-1.97383600
Cl	-0.82959000	-2.01349200	1.89723100
Cl	-0.75111600	1.92073800	-1.94010800
Cl	-0.19307000	2.16733400	2.00930200
Cl	3.11013700	0.23148100	-1.93034200
Cl	0.12498700	-1.67113700	-2.33009300
Cl	2.36862500	-0.47938500	2.31734000
C	1.15599700	-2.18027100	-1.03729800
C	1.75917600	-3.38870800	-1.10984400
B	2.74858400	-3.76709100	-0.04098600
N	1.35429000	-1.26137500	-0.01005000
C	-5.13091000	0.01744600	-0.04011100
C	-5.85478300	-0.20565300	1.13599200
C	-5.83491700	0.25691500	-1.22500300
C	-7.24231200	-0.18728300	1.12695300
H	-5.32681800	-0.36683400	2.07018400

C	-7.22249700	0.27038100	-1.23302500
H	-5.29221800	0.40508000	-2.15285900
C	-7.93112200	0.04963700	-0.05733000
H	-7.78756100	-0.35151000	2.05025800
H	-7.75242200	0.44648600	-2.16304500
H	-9.01574100	0.06195600	-0.06405900
Cl	3.83856400	5.08822200	0.12114900
Cl	3.61554700	-5.32366200	-0.06076600

BN-41-DPTTM-D₀

C	0.00336700	0.61173200	-0.00066300
C	1.25082900	-0.13414900	-0.00698200
C	1.47626600	-1.27162900	-0.81579400
C	2.34263400	0.22817100	0.81806100
C	2.67072200	-1.96650200	-0.81328000
C	3.54181100	-0.45505400	0.81954300
C	3.73127600	-1.56902400	0.00043500
H	2.76662100	-2.83512800	-1.45267400
H	4.33750600	-0.10893500	1.46724100
C	-0.04710600	2.06716400	0.00433500
C	0.79103300	2.84205900	-0.83257800
C	-0.92863300	2.81022700	0.82153300
C	0.77421100	4.22453200	-0.84289700
C	-0.96910900	4.19400200	0.81922500
C	-0.11040400	4.89291200	-0.01198200
H	1.42792500	4.76960800	-1.51033100
H	-1.65184100	4.71516100	1.47673900
C	-2.17488400	0.08029500	-1.00054600
C	-3.37164900	-0.54319100	-1.04615900
H	-3.98481000	-0.30286900	-1.90815700
H	-2.74174800	-2.41684800	1.91547600
Cl	0.27432000	-1.83293500	-1.93462100
Cl	2.20446200	1.53007100	1.95961900
Cl	1.84636600	2.09145700	-1.98409100
Cl	-1.97412100	2.03087800	1.96120500
Cl	-0.14617200	6.62230200	-0.01803400
Cl	-0.37230200	-1.14184600	2.29685700
Cl	-1.70649100	1.12608300	-2.30352600
C	-1.52129600	-1.03072200	1.00173000
C	-2.65405900	-1.76395300	1.05362000
B	-3.73918100	-1.57504300	0.00698400
N	-1.22376600	-0.10899600	-0.00013100
C	-5.09086600	-2.35888600	0.01242500

C	-6.18913300	-1.92832900	-0.74776600
C	-5.25962000	-3.52266700	0.77829500
C	-7.39504300	-2.61673800	-0.74123200
H	-6.10318400	-1.02795500	-1.34943800
C	-6.45730800	-4.22532100	0.78243600
H	-4.43210200	-3.89430100	1.37591900
C	-7.53071000	-3.77081000	0.02337000
H	-8.23038100	-2.25645800	-1.33336800
H	-6.55715500	-5.12676700	1.37879300
H	-8.47017300	-4.31444600	0.02758400
C	5.00932200	-2.30551600	-0.00145000
C	5.51655500	-2.85088300	-1.18564500
C	5.73971100	-2.47400700	1.17969500
C	6.71964400	-3.54243500	-1.18814800
H	4.97805200	-2.70860900	-2.11689600
C	6.94071900	-3.16922800	1.17616500
H	5.35022800	-2.08231200	2.11363700
C	7.43567500	-3.70503500	-0.00749300
H	7.10293300	-3.94962400	-2.11773900
H	7.48834300	-3.29952900	2.10352400
H	8.37526800	-4.24707400	-0.00977100

BN-41-metaDPTTM-D₀

C	0.00002900	0.59943700	0.00000300
C	-1.27824300	-0.09259400	0.00024800
C	-2.37845800	0.29222100	-0.79986200
C	-1.51776600	-1.21481200	0.82997400
C	-3.58624000	-0.37903300	-0.78587800
C	-2.71788900	-1.89623200	0.84261500
C	-3.77953200	-1.49183900	0.03207800
H	-4.38699200	-0.01845200	-1.41936500
H	-2.82152100	-2.75597500	1.49261100
C	1.27833200	-0.09253700	-0.00023100
C	1.51783100	-1.21482900	-0.82985600
C	2.37858400	0.29238100	0.79978100
C	2.71796500	-1.89623100	-0.84249900
C	3.58638300	-0.37884400	0.78578400
C	3.77964800	-1.49172700	-0.03207100
H	2.82157400	-2.75604700	-1.49240300
H	4.38716800	-0.01818300	1.41918500
C	0.62474200	2.74497200	-1.01568500
C	0.68669900	4.09516800	-1.07342700
H	1.19408800	4.52230200	-1.93015600

H	-1.19448900	4.52215600	1.93010300
Cl	-2.25803600	1.60993200	-1.92340800
Cl	-0.31909000	-1.76086600	1.96172600
Cl	0.31904300	-1.76106900	-1.96140000
Cl	2.25821400	1.61021300	1.92319100
Cl	-1.28403000	1.81238600	2.31569900
Cl	1.28389400	1.81256600	-2.31580400
C	-0.62489100	2.74489800	1.01564800
C	-0.68701600	4.09508600	1.07339100
B	-0.00019100	4.89469400	-0.00000800
N	-0.00002200	2.02742200	-0.00001100
C	-5.06545100	-2.21429000	0.04504200
C	-5.80619300	-2.37552200	-1.13066500
C	-5.57016500	-2.75294600	1.23336700
C	-7.01490500	-3.05713500	-1.11785500
H	-5.41917200	-1.98826600	-2.06748400
C	-6.78095000	-3.43081100	1.24516300
H	-5.02400200	-2.61552200	2.16085300
C	-7.50724700	-3.58636300	0.06983500
H	-7.57085600	-3.18162700	-2.04103900
H	-7.16235500	-3.83245400	2.17793300
H	-8.45298200	-4.11752500	0.07946800
Cl	-0.00032000	6.67770900	-0.00002100
C	5.06557900	-2.21415300	-0.04503600
C	5.80655600	-2.37494800	1.13058300
C	5.57006700	-2.75321900	-1.23326900
C	7.01528100	-3.05653900	1.11777600
H	5.41971100	-1.98736000	2.06733800
C	6.78086500	-3.43106100	-1.24506300
H	5.02371200	-2.61613900	-2.16069400
C	7.50739900	-3.58617800	-0.06982400
H	7.57141900	-3.18068700	2.04089300
H	7.16209400	-3.83302800	-2.17776600
H	8.45314300	-4.11732400	-0.07945700

BN-41-TPTTM-D₀

C	-0.00510000	0.01801900	-0.00197800
C	-1.34613900	0.58004300	0.00469400
C	-2.39535400	0.09024600	0.81555400
C	-1.70334400	1.67024300	-0.82466400
C	-3.66392400	0.63861200	0.81147200
C	-2.96522800	2.22959200	-0.82798100
C	-3.97394700	1.72443100	-0.00667600

H	-4.41923200	0.20257100	1.45331100
H	-3.15936500	3.07268700	-1.47907600
C	1.19650700	0.83689300	-0.00964000
C	1.32872500	1.97775200	0.81792300
C	2.32308400	0.56439900	-0.81878900
C	2.45477400	2.77597400	0.82239800
C	3.45803800	1.35298600	-0.81326600
C	3.54560900	2.47924300	0.00427900
H	2.47654800	3.64192000	1.47205400
H	4.28581900	1.07443600	-1.45338900
C	0.85038900	-2.05193600	1.00372200
C	1.05229600	-3.38642600	1.05390700
H	1.60653800	-3.73737300	1.91789400
H	-0.82252600	-3.99102700	-1.91183000
Cl	-2.13380500	-1.20548600	1.94053000
Cl	-0.57402900	2.32937700	-1.96798200
Cl	0.08889300	2.40181300	1.95807700
Cl	2.32468600	-0.75802100	-1.94310600
Cl	-1.18706000	-1.32571500	-2.30180300
Cl	1.41791900	-1.05309800	2.30406900
C	-0.42568700	-2.18520100	-1.00104100
C	-0.35057100	-3.53288600	-1.04918500
B	0.43779300	-4.29426100	0.00245800
N	0.13865400	-1.39892200	0.00037100
C	0.60006800	-5.84892300	0.00273600
C	1.59815000	-6.48022200	0.76072300
C	-0.24508700	-6.67369500	-0.75534300
C	1.75136900	-7.86041900	0.75956700
H	2.27867900	-5.87783500	1.35579600
C	-0.10834500	-8.05562400	-0.75407500
H	-1.03565600	-6.22584300	-1.35079000
C	0.89441600	-8.65277200	0.00280500
H	2.53732300	-8.32106400	1.34979600
H	-0.78143100	-8.66947400	-1.34435600
H	1.00771600	-9.73229300	0.00280400
C	-5.32524700	2.31625200	-0.00770200
C	-6.06521500	2.40859900	1.17587200
C	-5.89439600	2.79708200	-1.19167600
C	-7.33579000	2.96671600	1.17498200
H	-5.63089800	2.06572100	2.10926700
C	-7.16659100	3.35150600	-1.19158600
H	-5.34753300	2.71058100	-2.12489400
C	-7.89171200	3.43927900	-0.00853900
H	-7.89083400	3.03946100	2.10426200

H	-7.59630700	3.70937400	-2.12121200
H	-8.88556100	3.87395200	-0.00892100
C	4.75354000	3.32607400	0.00834800
C	5.46672500	3.55884000	-1.17239200
C	5.21080500	3.91349600	1.19278500
C	6.60214500	4.35674700	-1.16833700
H	5.11374700	3.13375900	-2.10627400
C	6.34837000	4.70834300	1.19583100
H	4.68749600	3.72337100	2.12418200
C	7.04774900	4.93381200	0.01551900
H	7.13670600	4.53444300	-2.09548000
H	6.69428800	5.14698100	2.12581600
H	7.93619300	5.55618700	0.01833500

The Cartesian coordinates of periphery-engineered radicals at their lowest excited state geometries.

BN-41-MPTTM-D₁

C	-0.70657000	-0.00209200	-0.00367600
C	-1.31057400	1.30115300	-0.03815200
C	-0.83828200	2.40468600	-0.79596200
C	-2.44782200	1.62738300	0.75603900
C	-1.40646200	3.66546100	-0.78018600
C	-3.06316400	2.86614300	0.75860200
C	-2.53191100	3.88979100	-0.00636200
H	-0.99281400	4.45081200	-1.39884400
H	-3.92742800	3.03581400	1.38705000
C	-1.41583700	-1.24673100	0.03668900
C	-2.59220000	-1.46569900	-0.73967500
C	-1.02861900	-2.39633900	0.77476500
C	-3.31019300	-2.64711500	-0.74498700
C	-1.70248000	-3.60367200	0.75450900
C	-2.85631200	-3.72197400	-0.00037000
H	-4.19506000	-2.73495400	-1.36139400
H	-1.34519600	-4.42985800	1.35476900
C	1.45964500	-0.67274900	-1.03726700
C	2.80496500	-0.79123000	-1.07762200
H	3.19560600	-1.33760600	-1.92832100
H	3.23056800	1.21795700	1.84557500
Cl	0.48986200	2.20673600	-1.91148400
Cl	-3.27518000	5.46063300	0.00819500

Cl	-3.11054700	0.46155600	1.86388600
Cl	-3.16440200	-0.24170300	-1.83427700
Cl	0.33092800	-2.33757300	1.87121400
Cl	-3.73070400	-5.22331900	-0.01878400
Cl	0.57895100	1.14084200	2.34981200
Cl	0.50113300	-1.31047500	-2.31067200
C	1.43202100	0.52468100	1.01109300
C	2.83141600	0.62454800	1.03113300
B	3.66184900	-0.10592900	-0.02773600
N	0.73793500	-0.04669500	0.00820400
C	5.20374800	-0.10041400	-0.00709800
C	5.95136800	-0.81588100	-0.97294100
C	5.92990800	0.61483000	0.97704400
C	7.33084800	-0.81914700	-0.95697300
H	5.42980900	-1.37758900	-1.73993200
C	7.31095800	0.61556100	0.99690400
H	5.39556800	1.17978600	1.73284400
C	8.01532800	-0.10187500	0.02946200
H	7.88664800	-1.37465900	-1.70391200
H	7.84810500	1.17034400	1.75780400
H	9.10003800	-0.10330500	0.04164100

BN-41-metaMPTTM-D₁

C	0.65934500	-0.09078300	0.00443000
C	-0.77866400	-0.10887200	-0.04171300
C	-1.55938000	0.44816400	-1.11062000
C	-1.58078600	-0.64807900	1.03634600
C	-2.92421200	0.48001200	-1.10215500
C	-2.94461800	-0.65258800	1.02979300
C	-3.68597700	-0.07647400	-0.03406100
H	-3.42158400	0.88422400	-1.97343500
H	-3.45141900	-1.04485100	1.90096100
C	1.45672600	-1.19084500	0.46188100
C	1.11970800	-2.53739600	0.14002900
C	2.64646600	-1.06126600	1.23161900
C	1.84784400	-3.63286400	0.55751300
C	3.40167800	-2.14231700	1.64057800
C	2.99671300	-3.42800300	1.30638700
H	1.54207500	-4.63037900	0.27148600
H	4.28483100	-1.98281500	2.24498900
C	2.25403500	1.06822900	-1.46430100
C	2.95279600	2.14551900	-1.89760700
H	3.64324900	1.98071700	-2.71618400

H	1.34254600	4.37290900	0.38123600
Cl	-0.77935600	1.02750600	-2.54716200
Cl	-0.80214400	-1.24964100	2.46198400
Cl	-0.22592200	-2.86023500	-0.90474900
Cl	3.17010800	0.48713400	1.81090600
Cl	-0.03254300	2.27345400	1.50832800
Cl	2.46079800	-0.45208500	-2.26491500
C	1.06758300	2.32001100	0.17094100
C	1.63785200	3.49579300	-0.18212600
B	2.67412100	3.48411000	-1.27211800
N	1.32295000	1.09514000	-0.43231200
C	-5.11997800	-0.05182600	-0.03932700
C	-5.84665400	0.78540000	-0.93349100
C	-5.87979600	-0.86290100	0.85099600
C	-7.22385400	0.80762200	-0.93065800
H	-5.31580000	1.44398000	-1.60946900
C	-7.25622400	-0.83588700	0.84236300
H	-5.37426000	-1.53951400	1.52864100
C	-7.94585900	-0.00126400	-0.04592500
H	-7.75020600	1.46384100	-1.61499500
H	-7.80892300	-1.47314300	1.52387200
H	-9.02975300	0.01743500	-0.04838400
Cl	3.93647300	-4.78436500	1.82666900
Cl	3.51674000	4.96944400	-1.79448300

BN-41-DPTTM-D₁

C	-0.01261800	0.63173200	0.02099800
C	-1.25613700	-0.08692100	0.04896100
C	-1.49179600	-1.26289500	0.84194500
C	-2.38714600	0.28751800	-0.77343700
C	-2.66345600	-1.96150500	0.81454500
C	-3.57043800	-0.38928700	-0.77881800
C	-3.76715200	-1.55560000	0.00796500
H	-2.75811900	-2.80746000	1.48175500
H	-4.33972800	-0.05287700	-1.46036200
C	0.07753500	2.06441500	-0.00900000
C	-0.78989900	2.88258700	0.76927800
C	1.03178900	2.79289600	-0.77173900
C	-0.74531300	4.26199800	0.77255200
C	1.10695600	4.17192800	-0.76738100
C	0.21329100	4.90364300	0.00275800
H	-1.42722900	4.82687600	1.39399800
H	1.83925300	4.67250700	-1.38691300

C	2.16970900	0.06980700	1.00200900
C	3.36677700	-0.56106200	1.02409300
H	4.00285300	-0.31565400	1.86793800
H	2.63882600	-2.48775400	-1.88158500
Cl	-0.29698300	-1.79690600	1.98058800
Cl	-2.23288200	1.60216200	-1.89252100
Cl	-1.92647100	2.14740000	1.85320800
Cl	2.10703600	1.98141200	-1.86336900
Cl	0.29847200	6.63245600	0.00339500
Cl	0.25941700	-1.19117000	-2.20477900
Cl	1.74353100	1.13881200	2.30011900
C	1.46465500	-1.06124600	-0.96129100
C	2.58559400	-1.81214300	-1.03446500
B	3.70070700	-1.60878700	-0.02344700
N	1.19658400	-0.12009800	0.02712700
C	5.04920700	-2.39950500	-0.05362300
C	6.17073600	-1.96176700	0.66797100
C	5.19243400	-3.57667000	-0.80446000
C	7.37309800	-2.65575300	0.63933900
H	6.10528300	-1.05090600	1.25629000
C	6.38676300	-4.28446600	-0.83101700
H	4.34696600	-3.95421700	-1.37258100
C	7.48305900	-3.82280000	-0.10972200
H	8.22610900	-2.28941200	1.20191400
H	6.46627500	-5.19576000	-1.41546600
H	8.41992800	-4.37052300	-0.13140900
C	-4.99989500	-2.28652200	-0.00659400
C	-5.09507300	-3.59819100	0.54133600
C	-6.18564800	-1.73425700	-0.57066800
C	-6.28211400	-4.29669100	0.52170400
H	-4.21587000	-4.07608900	0.95497800
C	-7.36779300	-2.44004600	-0.58122400
H	-6.17389700	-0.72903000	-0.97311500
C	-7.43264700	-3.72888200	-0.03724800
H	-6.32077100	-5.29791100	0.93676500
H	-8.25700200	-1.98873100	-1.00768900
H	-8.36540000	-4.28116500	-0.04868500

BN-41-metaDPTM-D₁

C	-0.00097600	0.56243100	-0.01178400
C	1.27271100	-0.08096700	0.01085100
C	2.41430300	0.38233900	0.73815900
C	1.53932000	-1.26283700	-0.76554600

C	3.62521900	-0.26222500	0.72241400
C	2.74719700	-1.91260600	-0.77715000
C	3.83629200	-1.43428300	-0.03215400
H	4.43010100	0.15754900	1.31203600
H	2.84379900	-2.80568700	-1.38082300
C	-1.25229000	-0.12716900	-0.03512200
C	-1.48827300	-1.31531100	0.75494700
C	-2.40855900	0.30058000	-0.76833200
C	-2.67551000	-1.99357800	0.77014800
C	-3.60592600	-0.35982600	-0.72959900
C	-3.78963500	-1.53950500	0.03480600
H	-2.76516300	-2.84928500	1.42636800
H	-4.40351000	0.00463800	-1.36389300
C	-0.67693300	2.69061400	1.00600500
C	-0.77966300	4.03962100	1.07263500
H	-1.31143800	4.44879600	1.92329800
H	1.13066000	4.52847600	-1.90325800
Cl	2.29462400	1.75291400	1.79850400
Cl	0.31073900	-1.88600500	-1.81913500
Cl	-0.25232100	-1.88161700	1.82871800
Cl	-2.30329700	1.63353900	-1.87553000
Cl	1.28819900	1.81465200	-2.29659600
Cl	-1.33368900	1.72336200	2.28376400
C	0.58097000	2.73074300	-1.00890400
C	0.61792100	4.08431700	-1.05847700
B	-0.09996500	4.85922000	0.01111900
N	-0.03212900	1.99165900	-0.00561800
C	5.13103400	-2.10864000	-0.04242800
C	6.02620700	-1.97991100	1.03579100
C	5.52465200	-2.91022900	-1.12996900
C	7.25083800	-2.62534300	1.02723400
H	5.74470300	-1.39512400	1.90422400
C	6.75237000	-3.54907700	-1.13752900
H	4.87492900	-3.00548300	-1.99267400
C	7.62356300	-3.41291200	-0.05906200
H	7.91751600	-2.52045100	1.87648500
H	7.03809800	-4.15074400	-1.99373700
H	8.58466300	-3.91526200	-0.06599200
Cl	-0.14289100	6.64584400	0.02081200
C	-5.05836300	-2.23588900	0.05860600
C	-6.26123400	-1.58245700	-0.29467700
C	-5.14030400	-3.59510500	0.43858100
C	-7.47072400	-2.24939200	-0.26465400
H	-6.24661500	-0.53214000	-0.56102900

C	-6.35214600	-4.25708500	0.46248600
H	-4.23671100	-4.14117600	0.68318100
C	-7.52788900	-3.59124600	0.11269000
H	-8.38052400	-1.72125500	-0.52866100
H	-6.38590500	-5.30342700	0.74613000
H	-8.47809300	-4.11314200	0.13316700

BN-41-TPTTM-D₁

C	0.01117300	-0.05154800	-0.01274800
C	-1.16222300	-0.86782000	-0.03906100
C	-2.34822800	-0.56696800	-0.79231200
C	-1.28441500	-2.06877400	0.76008500
C	-3.47043400	-1.34555500	-0.76338700
C	-2.39548000	-2.86223300	0.76867600
C	-3.54396400	-2.53403500	0.01170500
H	-4.29147300	-1.06886800	-1.41159800
H	-2.40494400	-3.71509000	1.43426500
C	1.34386900	-0.56377700	0.01651700
C	1.73223500	-1.70997100	-0.75483500
C	2.42389600	0.01142700	0.75547000
C	3.00162800	-2.23276700	-0.75899800
C	3.69599500	-0.50620400	0.74938900
C	4.02837200	-1.64596200	-0.00510700
H	3.19565100	-3.11119300	-1.36114100
H	4.45084500	-0.00929300	1.34553800
C	0.39377300	2.16425000	-1.00459200
C	0.30445200	3.51360000	-1.04452500
H	0.78208700	3.98463900	-1.89709000
H	-1.70146900	3.66898900	1.89408600
Cl	-2.36339500	0.76286800	-1.90759700
Cl	-0.01072700	-2.49829300	1.85403100
Cl	0.58068000	-2.45808100	-1.81602500
Cl	2.15454200	1.35897100	1.81756800
Cl	-1.47440500	0.97313800	2.25283700
Cl	1.18925900	1.32000900	-2.29548300
C	-0.89410600	2.00269600	0.98062800
C	-1.12305200	3.33380800	1.03966400
B	-0.50501300	4.25585300	0.00362700
N	-0.16403200	1.36417600	-0.01463500
C	-0.68553200	5.81005200	0.01338600
C	0.15699400	6.64989400	-0.73096500
C	-1.69675000	6.42582800	0.76669400
C	0.00492000	8.03029600	-0.72186600

H	0.95777300	6.21478400	-1.32221100
C	-1.86478600	7.80439900	0.77426100
H	-2.37556100	5.81196400	1.35197700
C	-1.01049000	8.61169800	0.03037500
H	0.67646100	8.65527100	-1.30227800
H	-2.66055600	8.25213400	1.36140600
H	-1.13549800	9.68992500	0.03693400
C	-4.72918700	-3.35631700	0.02465000
C	-5.98277000	-2.85020800	-0.39909900
C	-4.68606500	-4.70294500	0.46267900
C	-7.11505700	-3.63961800	-0.38085400
H	-6.06926800	-1.81673600	-0.71241300
C	-5.82159300	-5.48704800	0.47350700
H	-3.74210100	-5.14158500	0.76348100
C	-7.04718200	-4.96465500	0.05376200
H	-8.06401300	-3.22204400	-0.69955200
H	-5.75707300	-6.51865500	0.80231800
H	-7.93765800	-5.58308600	0.06453600
C	5.38790000	-2.18766000	-0.00657400
C	6.23517900	-2.02057400	1.10178900
C	5.88612900	-2.89152100	-1.11581200
C	7.52026100	-2.53803900	1.10093300
H	5.87141900	-1.50848700	1.98583200
C	7.17328100	-3.40330800	-1.11559700
H	5.26936100	-3.00916600	-2.00003400
C	7.99819000	-3.23139900	-0.00734600
H	8.15120800	-2.40683100	1.97361800
H	7.53989500	-3.93209700	-1.98903300
H	9.00538400	-3.63371900	-0.00791900