

Classification of EWG-/EDG- characteristics of substituents according to Hammett constants:

Electronic characterization of the substituents used in this study is provided in the following table (Hammett constants - σ_p):

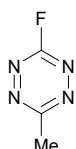
Entry	σ_p	R ¹	R ² = Ph			R ² = Me		
			E(LUMO) [eV]	E(LUMO+1) [eV]	ΔG^\ddagger kJ/mol	E(LUMO) [eV]	E(LUMO+1) [eV]	ΔG^\ddagger kJ/mol
1	0.54	CF ₃	-0.0891	-0.0726	54.1	-0.0918	-0.0540	57.4
2	0.1	SeMe	-0.0701	-0.0481	75.5	-0.0697	-0.0230	79.2
3	0.19	NCO	-0.0814	-0.0613	65.9	-0.0823	-0.0418	69.8
4	0.72	SO₂Me	-0.0917	-0.0755	41.5	-0.0945	-0.0561	42.8
5	0.49	SOMe	-0.0843	-0.0651	47.2	-0.0861	-0.0454	52.6
6	0.08	N ₃	-0.0790	-0.0585	70.3	-0.0792	-0.0407	73.6
7	0.15	SMe	-0.0699	-0.0472	75.2	-0.0693	-0.0217	79.0
8	0.52	SCN	-0.0922	-0.0683	56.6	-0.0943	-0.0487	60.2
9	-0.66	NH ₂	-0.0633	-0.0308	87.0	-0.0611	0.0008	90.7
10	0.23	Br	-0.0834	-0.0613	64.1	-0.0850	-0.0393	67.4
11	0.49	NC	-0.0913	-0.0796	53.0	-0.0940	-0.0662	58.9
12	0.23	Cl	-0.0838	-0.0606	62.9	-0.0852	-0.0382	66.6
13	0.66	CN	-0.0940	-0.0882	52.4	-0.0979	-0.0763	54.7
14	0.06	F	-0.0873	-0.0546	60.9	-0.0883	-0.0279	65.0

Hammett constants were obtained from previously published data.¹

Literature:

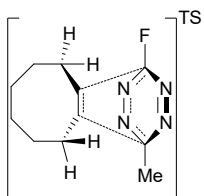
1 – C. R. Hansch, A. Leo and R. W. Taft, *Chem. Rev.*, 1991, **91**, 165-1195.

Coordinates of optimised structures:

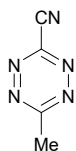


C	1.29837900	0.00000600	-0.00251400
C	-1.22441700	0.00003500	0.00900600
N	-0.59677100	1.18524600	0.01191400
N	-0.59678200	-1.18521600	0.01191200
N	0.71461900	1.18759200	0.00550800
N	0.71457700	-1.18759300	0.00550900
F	2.61118000	-0.00002800	-0.01350800

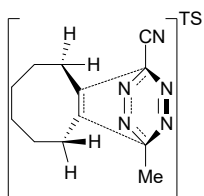
C	-2.71967400	-0.00000600	-0.01229400
H	-3.07649600	-0.00161300	-1.04701900
H	-3.09968800	-0.89522000	0.48108800
H	-3.09966400	0.89667500	0.47841600



C	-1.81540800	-1.20009600	0.33939000
C	-1.85858000	1.15815300	-0.37736400
N	-2.11291400	0.22290500	-1.33684800
N	-2.17089100	0.91230600	0.92549800
N	-2.10484900	-1.01149600	-0.96309100
C	0.37142000	-0.66154100	0.29146000
C	0.96173100	-1.79803500	-0.49027500
C	2.36244600	1.27522600	1.13916800
C	2.49874300	-1.67838500	-0.32665800
C	3.38777400	0.81010900	0.08836200
C	3.09098400	-0.36318200	-0.88089800
H	0.69740800	-1.71023300	-1.55104100
H	2.75655200	-1.79359000	0.73465600
H	2.20727500	0.46912800	1.86570700
H	4.29489200	0.55024900	0.64874100
H	0.61408200	-2.77085700	-0.13195500
H	2.81756100	2.10198400	1.69818100
H	2.95944300	-2.52641200	-0.84505700
H	3.66380700	1.67207100	-0.53358400
H	4.05325100	-0.59882400	-1.34983100
H	2.45676000	-0.01489100	-1.70383400
C	0.40770400	0.60801400	-0.21433300
C	0.97510000	1.72337900	0.62817600
H	1.05834200	2.64545900	0.04295800
H	0.33045900	1.93431100	1.49140600
H	0.44109200	-0.76708300	1.37638200
H	0.48726900	0.71209300	-1.29578800
N	-2.16330100	-0.32317900	1.30010300
F	-1.68739300	-2.45838800	0.72673900
C	-1.78919900	2.58922500	-0.81314200
H	-2.79186900	2.94954700	-1.06183800
H	-1.39003900	3.20622700	-0.00668000
H	-1.16236000	2.68536200	-1.70203600

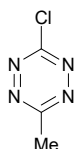


C	0.98409500	-0.00001800	0.00126100
C	-1.55553600	0.00008900	0.00871500
N	-0.92901200	1.18823700	0.01329200
N	-0.92905200	-1.18815500	0.01329400
N	0.37917500	1.19232600	0.00866100
N	0.37906500	-1.19235800	0.00866000
C	2.42994300	-0.00006300	-0.00793000
N	3.58446200	-0.00000200	-0.01432300
C	-3.04797800	0.00000200	-0.01728400
H	-3.39516400	-0.00358200	-1.05582700
H	-3.43022700	-0.89594000	0.47302300
H	-3.43021400	0.89911300	0.46713900

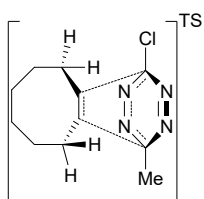


C	1.99940700	0.76013800	0.17103900
C	1.53315600	-1.62501200	-0.33955100
N	1.93584000	-0.84338500	-1.38492000
N	1.94945800	-1.34444100	0.92919000
N	2.17442200	0.39391400	-1.12820900
C	-0.35012700	0.62687300	0.19892200
C	-0.78456200	1.74712200	-0.69652300
C	-2.57352600	-0.88348100	1.28276700
C	-2.31959400	1.87377200	-0.50089300
C	-3.55363700	-0.38966000	0.20284800
C	-3.11795700	0.61226400	-0.89706800
H	-0.56764200	1.50640000	-1.74431000
H	-2.52588600	2.14283500	0.54343700
H	-2.27714400	-0.03491600	1.91047600
H	-4.39363300	0.06347500	0.74430200
H	-0.29812600	2.69577800	-0.45161000
H	-3.12564400	-1.56616800	1.94002200
H	-2.66099200	2.72074400	-1.10552600
H	-3.97356400	-1.26382000	-0.31225200
H	-4.04891700	0.94002700	-1.37349900
H	-2.57083000	0.08515400	-1.68674600
C	-0.58146000	-0.67066600	-0.16752800
C	-1.28688600	-1.58959000	0.80201100
H	-1.52983600	-2.54217400	0.31940400
H	-0.65475800	-1.80907900	1.67215100

H	-0.35058500	0.85444800	1.26727800
H	-0.72530000	-0.86533200	-1.22957800
N	2.18552500	-0.10860400	1.20058700
C	2.12519400	2.16663700	0.47744600
N	2.17049300	3.29532600	0.72047300
C	1.16515600	-3.04212700	-0.64627500
H	2.07043900	-3.60179500	-0.90120400
H	0.70418100	-3.50793700	0.22560800
H	0.48710400	-3.08491900	-1.50097900

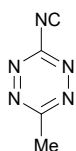


C	0.88693700	0.00008000	0.00218400
C	-1.65038600	0.00012400	0.00851600
N	-1.02288200	1.18498600	0.01376800
N	-1.02283300	-1.18488100	0.01375900
N	0.28798300	1.18860800	0.01003400
N	0.28787800	-1.18856100	0.01004600
Cl	2.60517400	-0.00006500	-0.01054400
C	-3.14479800	-0.00007200	-0.01787100
H	-3.49613300	-0.00510600	-1.05465900
H	-3.52667200	-0.89427400	0.47600400
H	-3.52668700	0.89862600	0.46769300

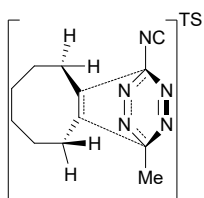


C	1.95599600	-0.58391000	-0.15331100
C	1.30411700	1.75121400	0.37314200
N	1.75849700	0.99198200	1.41332000
N	1.74814100	1.51295300	-0.89443600
N	2.10288300	-0.21939200	1.14403300
C	-0.36310600	-0.60763600	-0.17609400
C	-0.73823400	-1.73646200	0.73584600
C	-2.68395600	0.71866000	-1.31425300
C	-2.25502500	-1.98179000	0.51880000
C	-3.64334400	0.17146700	-0.24155600
C	-3.15438700	-0.77929300	0.88117600
H	-0.55782900	-1.45816500	1.78134000
H	-2.42323500	-2.28117200	-0.52430700
H	-2.31567500	-0.11597500	-1.92227900
H	-4.43948800	-0.34989100	-0.78808400

H	-0.17896100	-2.65168600	0.52401500
H	-3.27401300	1.34817900	-1.99151700
H	-2.54348700	-2.84265100	1.13180600
H	-4.13385700	1.02065300	0.25265900
H	-4.06702800	-1.17030000	1.34544900
H	-2.66384800	-0.20168900	1.67262100
C	-0.70499000	0.67301200	0.16665500
C	-1.46070900	1.52421100	-0.82581300
H	-1.78038900	2.46345700	-0.36181600
H	-0.83220800	1.77667400	-1.68943100
H	-0.33648400	-0.85387900	-1.23972100
H	-0.89041800	0.86641900	1.22231800
N	2.08895200	0.30141300	-1.17014600
Cl	2.33176600	-2.22923600	-0.53639400
C	0.85250100	3.14330400	0.69145600
H	1.71866300	3.75329100	0.96495900
H	0.37511900	3.59101100	-0.18122000
H	0.16062300	3.13736900	1.53622100

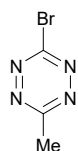


C	1.01340100	0.00002500	0.00173600
C	-1.52385100	0.00006300	0.00831600
N	-0.89582400	1.18608500	0.01295100
N	-0.89582700	-1.18601600	0.01295300
N	0.41229600	1.19188100	0.00897300
N	0.41224100	-1.19185900	0.00897200
N	2.38720400	-0.00002000	-0.00767400
C	3.56531600	-0.00006500	-0.01648800
C	-3.01730600	-0.00002900	-0.01728000
H	-3.39900600	0.89849900	0.46870500
H	-3.36792200	-0.00373400	-1.05446100
H	-3.39906200	-0.89522500	0.47482600

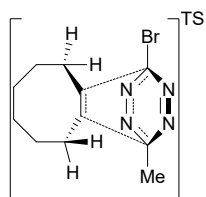


C	1.96995900	0.80603100	0.18915300
C	1.55080300	-1.57916700	-0.34637200
N	1.94469500	-0.77885600	-1.38056700
N	1.95316700	-1.30154800	0.92722100
N	2.16599900	0.45873400	-1.11014900
C	-0.34909600	0.62281400	0.20302000

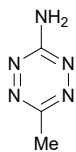
C	-0.79874200	1.74701100	-0.67915400
C	-2.55916700	-0.92324300	1.26902400
C	-2.33434000	1.85731400	-0.48093700
C	-3.54487300	-0.42684800	0.19545100
C	-3.11972100	0.59252100	-0.89235200
H	-0.58069800	1.52082200	-1.72993400
H	-2.54268400	2.11089800	0.56690900
H	-2.27144700	-0.07900400	1.90648900
H	-4.38939700	0.01107500	0.74242600
H	-0.32090400	2.69758900	-0.42433500
H	-3.10401000	-1.61924600	1.91838100
H	-2.68522400	2.70810800	-1.07480100
H	-3.95584900	-1.29906300	-0.33007100
H	-4.05394700	0.91592600	-1.36541000
H	-2.56655600	0.08043400	-1.68767600
C	-0.56869500	-0.67298900	-0.17780200
C	-1.26530000	-1.61025000	0.78023900
H	-1.49761600	-2.56008700	0.28702300
H	-0.63096700	-1.83238500	1.64807100
H	-0.35507800	0.83910300	1.27369000
H	-0.70937700	-0.85795200	-1.24199700
N	2.17191700	-0.06529100	1.21076400
N	2.08215100	2.14610500	0.49358600
C	2.12535800	3.29565500	0.74062300
C	1.22321500	-3.00340400	-0.67005300
H	0.54891600	-3.05512500	-1.52730600
H	2.14281100	-3.53785600	-0.92719900
H	0.77012600	-3.48991800	0.19470900



C	0.26563400	0.00016300	0.00614800
C	-2.27242300	0.00018100	0.00815500
N	-1.64543100	1.18521800	0.01508000
N	-1.64531100	-1.18504600	0.01506700
N	-0.33400900	1.18834600	0.01351500
N	-0.33412300	-1.18822100	0.01353700
Br	2.13622400	-0.00005500	-0.00644400
C	-3.76672700	-0.00014900	-0.02223200
H	-4.11500900	-0.00841700	-1.06005400
H	-4.14981000	-0.89299700	0.47321700
H	-4.14980300	0.90007900	0.45956900

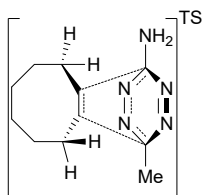


C	1.65693300	0.31076900	-0.01063400
C	0.22891400	2.30581000	0.34779800
N	0.86504700	1.80214900	1.44611400
N	0.78784100	2.17125700	-0.88922800
N	1.61259700	0.76837900	1.26415500
C	-0.50751100	-0.51170900	-0.08688800
C	-0.53120300	-1.63961900	0.89977900
C	-3.06422200	-0.13312400	-1.40844100
C	-1.85724500	-2.40481700	0.64933400
C	-3.84444300	-0.91170000	-0.33338600
C	-3.13269700	-1.56426200	0.87938400
H	-0.52131000	-1.24857500	1.92458000
H	-1.84871200	-2.81078800	-0.37104900
H	-2.39627400	-0.82475200	-1.93500900
H	-4.37810500	-1.70838600	-0.86713700
H	0.32063000	-2.31428900	0.78227800
H	-3.79014300	0.21249200	-2.15459800
H	-1.87311800	-3.27073700	1.32019600
H	-4.62608500	-0.25589600	0.07273200
H	-3.88544200	-2.21504200	1.33901700
H	-2.91809600	-0.80486200	1.63960700
C	-1.28292800	0.59284600	0.14322400
C	-2.22143600	1.07214800	-0.93829100
H	-2.86987100	1.86928900	-0.55900800
H	-1.66568100	1.47463500	-1.79481100
H	-0.33637000	-0.80267200	-1.12547800
H	-1.58550500	0.77442900	1.17356700
N	1.53006700	1.13477100	-1.07847700
Br	2.65676100	-1.25814300	-0.30682700
C	-0.68766100	3.47033800	0.56392900
H	-0.09820200	4.35449600	0.82461300
H	-1.24519400	3.68249400	-0.34935300
H	-1.37702500	3.26719700	1.38602200



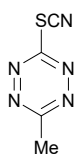
C	1.30148200	0.00004100	-0.00678100
C	-1.25565200	0.00005400	0.00760700
N	-0.62505300	1.18230500	0.03157600
N	-0.62502700	-1.18225900	0.03156700

N	0.68078300	1.19365300	0.02758500
N	0.68074800	-1.19361600	0.02764400
N	2.65431500	-0.00004000	-0.09259700
H	3.12925400	0.86653000	0.11143500
H	3.12898900	-0.86687100	0.11096500
C	-2.75204400	-0.00003900	-0.03859500
H	-3.14029500	0.89594200	0.44788200
H	-3.10060300	-0.00264300	-1.07635100
H	-3.14042400	-0.89359900	0.45224600

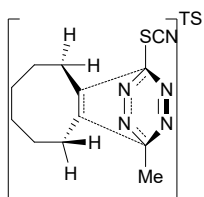


C	1.89524600	1.15492900	0.31216300
C	1.68606400	-1.24192600	-0.37444800
N	2.02451500	-0.34553900	-1.35810600
N	2.07433500	-1.00548300	0.91900100
N	2.13017200	0.88230600	-1.01402200
C	-0.29686700	0.68116000	0.29192500
C	-0.89361900	1.80954100	-0.49646100
C	-2.38597100	-1.15998600	1.16760900
C	-2.43194600	1.74192300	-0.33059500
C	-3.40032500	-0.70164300	0.10561000
C	-3.06929600	0.44682200	-0.87935300
H	-0.63547100	1.70870900	-1.55815100
H	-2.68381700	1.86775500	0.73109400
H	-2.20489300	-0.33480100	1.86669600
H	-4.30496900	-0.41145400	0.65522700
H	-0.53435400	2.78605100	-0.15142900
H	-2.86393100	-1.95317300	1.75576800
H	-2.86560100	2.60377300	-0.85025100
H	-3.68968200	-1.57088100	-0.49989100
H	-4.02274400	0.71192200	-1.35055000
H	-2.44648200	0.07015300	-1.69805500
C	-0.38278300	-0.60460400	-0.19563500
C	-1.01937400	-1.67082700	0.66868200
H	-1.14278600	-2.60060000	0.10277200
H	-0.38584600	-1.89343500	1.53668500
H	-0.35959100	0.79748400	1.37626400
H	-0.52847100	-0.70712600	-1.27013500
N	2.18259200	0.22030700	1.27579000
N	2.00259400	2.47371200	0.68932800
H	1.70452100	3.13941700	-0.01030500
H	1.69692600	2.67455200	1.63170800
C	1.57944900	-2.67957300	-0.79420200

H	0.90539800	-2.78071400	-1.64814900
H	2.56332300	-3.05374700	-1.09182400
H	1.21555200	-3.28590500	0.03683000

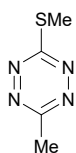


C	0.27331900	-0.40090900	0.00000200
C	-2.18601500	0.22123300	-0.00000700
N	-1.86926600	-1.08714500	-0.00000900
N	-1.28837800	1.21336500	-0.00002200
N	-0.60481900	-1.40878800	-0.00001100
N	-0.01319200	0.89401000	0.00000100
S	1.96062100	-0.96321300	0.00000700
C	2.76134100	0.53871500	0.00000200
N	3.39870500	1.50526500	0.00000000
C	-3.63706800	0.57776300	0.00001800
H	-4.12552400	0.15593900	-0.88223800
H	-4.12546000	0.15609300	0.88238500
H	-3.74977700	1.66161000	-0.00006400

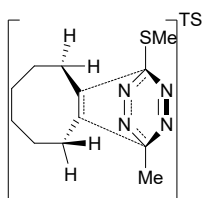


C	-1.86520700	0.19109800	-0.23319100
C	-0.59293800	2.31760400	-0.09658400
N	-1.11331300	1.99412100	-1.31605800
N	-1.20790000	1.89823500	1.04873500
N	-1.76964500	0.88786400	-1.39014800
C	0.38738100	-0.48008000	-0.08855700
C	0.55667000	-1.45810700	-1.21157600
C	2.84059700	-0.08206900	1.41081300
C	1.93968300	-2.12826000	-0.99404300
C	3.73601200	-0.62096600	0.28090200
C	3.13559500	-1.15263200	-1.04504400
H	0.54562200	-0.93945700	-2.17816500
H	1.92597400	-2.66709400	-0.03760700
H	2.22032000	-0.89954500	1.79619400
H	4.32312800	-1.43512500	0.72418200
H	-0.22258000	-2.22551300	-1.22648900
H	3.49719900	0.21414400	2.23784600
H	2.06345200	-2.89064500	-1.77077100
H	4.46496600	0.15517600	0.01223400
H	3.96240700	-1.66062400	-1.55446500

H	2.87661000	-0.31403200	-1.70129100
C	1.06287000	0.70993400	-0.11884800
C	1.90867600	1.10110200	1.07094800
H	2.49493400	1.99846900	0.84611600
H	1.28302100	1.32189400	1.94534000
H	0.20067500	-0.92321600	0.89220800
H	1.38329400	1.07318800	-1.09474700
N	-1.87590200	0.80014000	0.97817600
S	-2.78971800	-1.33242500	-0.42021100
C	-2.20692300	-2.13800600	0.96081000
N	-1.80715400	-2.73950700	1.86736400
C	0.22655400	3.56783900	-0.01667800
H	0.97954300	3.58278700	-0.80726800
H	-0.42507600	4.43665400	-0.15045900
H	0.70558300	3.64103200	0.96031300

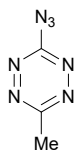


C	-0.51570900	-0.27708200	0.00009100
C	2.00832500	0.12019200	-0.00003300
N	1.56823700	-1.15600200	0.00008000
N	1.21043600	1.18647300	0.00014200
N	0.28572100	-1.36295500	0.00013900
N	-0.09275700	0.98594700	0.00020300
S	-2.23134700	-0.63641000	-0.00010100
C	-2.90163100	1.04801500	-0.00007600
H	-3.98673500	0.93352500	-0.00023200
H	-2.58364300	1.59063000	0.89013900
H	-2.58340100	1.59076000	-0.89012400
C	3.48842500	0.33435500	-0.00021000
H	3.93626500	-0.13091400	0.88192000
H	3.93607500	-0.13116000	-0.88230700
H	3.70507600	1.40259700	-0.00037000



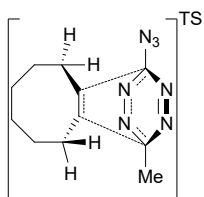
C	-1.85595100	-0.04719000	-0.20884200
C	-0.63035000	2.13032400	-0.28923000
N	-1.12297400	1.65542300	-1.48026300
N	-1.28040300	1.84010100	0.87520700
N	-1.74941000	0.53944500	-1.44360700
C	0.37608000	-0.56344800	-0.00901600

C	0.62788100	-1.59671000	-1.06491300
C	2.78395500	0.02703500	1.51590000
C	2.02720300	-2.19894500	-0.77539400
C	3.73029200	-0.54289200	0.44401400
C	3.18911100	-1.18464800	-0.85875700
H	0.62981000	-1.12996400	-2.05776800
H	2.01397000	-2.67964300	0.21221900
H	2.18819000	-0.79188500	1.93629400
H	4.34077400	-1.29987600	0.95278600
H	-0.12892500	-2.38614300	-1.06003200
H	3.40719100	0.39915900	2.33847400
H	2.20057300	-3.00176700	-1.50050600
H	4.43172700	0.24680700	0.14336500
H	4.04923900	-1.69338200	-1.30920600
H	2.91936300	-0.40241600	-1.57677200
C	1.00899400	0.65267900	-0.09745100
C	1.81480400	1.14652000	1.08239500
H	2.37157500	2.05121100	0.81502700
H	1.15937800	1.39816500	1.92582900
H	0.19415900	-0.95683600	0.99342000
H	1.36872200	0.93967100	-1.08443900
N	-1.90711000	0.71620200	0.91910500
S	-2.68679100	-1.60801200	-0.20943800
C	-2.85184200	-1.86545100	1.57804400
H	-3.30421300	-2.85151400	1.69659300
H	-1.87684300	-1.85161900	2.06901000
H	-3.48989100	-1.10209700	2.02108100
C	0.11978500	3.42771900	-0.34524600
H	0.91082800	3.38232600	-1.09713300
H	-0.56517500	4.23477000	-0.62157100
H	0.54770300	3.65507400	0.63222900

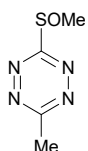


C	-0.57515800	0.44839800	-0.00003500
C	1.89328300	-0.17798100	0.00000100
N	1.00029500	-1.17054500	0.00003300
N	1.56818600	1.12962200	0.00003000
N	-0.27281600	-0.85065200	0.00000900
N	0.30892400	1.45930200	-0.00000500
N	-1.90877800	0.85008700	-0.00001700
N	-2.72624300	-0.09523600	0.00005200
N	-3.55988800	-0.84467600	-0.00003700
C	3.34762400	-0.52563200	-0.00001400
H	3.83520500	-0.10288600	-0.88235300

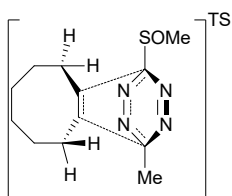
H	3.83544100	-0.10218700	0.88184700
H	3.46710800	-1.60896100	0.00034500



C	-1.86622300	0.10489100	0.46904200
C	-0.67417600	2.10384200	-0.41221100
N	-1.42546700	1.39745400	-1.30897300
N	-1.04530600	2.13959900	0.90636200
N	-2.04444800	0.36668600	-0.85662500
C	0.32268800	-0.50278500	0.37609200
C	0.28319800	-1.83019800	-0.32069400
C	3.04906000	0.26177100	1.04936800
C	1.70021500	-2.44813800	-0.19705300
C	3.68455800	-0.67955100	0.01095600
C	2.81750000	-1.61823700	-0.86541900
H	0.02992900	-1.70292400	-1.38075700
H	1.92800500	-2.60578900	0.86550000
H	2.55765700	-0.33972800	1.82325400
H	4.39031000	-1.30997900	0.56663800
H	-0.44526900	-2.51153900	0.13043300
H	3.86521500	0.79354300	1.55357300
H	1.66988700	-3.44405000	-0.65235800
H	4.30040600	-0.08069900	-0.67312000
H	3.52314800	-2.31594700	-1.33071000
H	2.38589300	-1.05762400	-1.70189500
C	0.94459700	0.56406200	-0.22393100
C	2.02779600	1.29729400	0.53369800
H	2.51984800	2.03127400	-0.11335000
H	1.60749800	1.83840500	1.39112700
H	0.36515200	-0.55670700	1.46569700
H	1.04484400	0.52884500	-1.30795200
N	-1.66107900	1.11235200	1.36560700
N	-2.45244400	-1.04764500	1.01885100
N	-2.92934300	-1.82798400	0.17407100
N	-3.39124500	-2.61485000	-0.48206500
C	0.07084800	3.29210200	-0.94154400
H	-0.64024700	4.07157100	-1.23081800
H	0.73036500	3.69435000	-0.17133200
H	0.65231100	3.01739600	-1.82434200

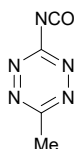


C	-0.24821200	-0.02672900	-0.18807600
C	2.27812400	-0.00508100	0.04055000
N	1.67574300	1.14525400	-0.29896200
N	1.63730800	-1.16434300	0.25804700
N	0.36984400	1.12776200	-0.42090100
N	0.33029300	-1.17853800	0.13743800
S	-2.05994200	-0.04154900	-0.44480400
O	-2.58648500	-1.32579400	0.10102100
C	-2.37839100	1.25778100	0.78751600
H	-3.45025300	1.45980900	0.75624000
H	-2.10069300	0.87692300	1.77268400
H	-1.80997100	2.15175200	0.52548400
C	3.76656200	-0.00588200	0.17667000
H	4.14804900	1.01028100	0.07895400
H	4.05304300	-0.42256000	1.14506600
H	4.20995700	-0.63654500	-0.59903300

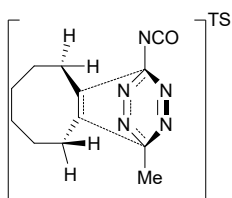


C	-1.66778100	0.19158400	-0.17541900
C	-0.39444200	2.31972400	-0.29315400
N	-0.92777600	1.86589700	-1.45963700
N	-0.99137500	2.03392100	0.89920000
N	-1.58810800	0.75547300	-1.39857700
C	0.56474100	-0.53526300	0.00294100
C	0.70984200	-1.61281500	-1.03084300
C	3.00940800	-0.04236700	1.47988200
C	2.08085000	-2.28382200	-0.74555900
C	3.89824100	-0.70200800	0.40944600
C	3.29654600	-1.33917100	-0.86944900
H	0.70841300	-1.18885700	-2.04247700
H	2.04860300	-2.73636100	0.25395200
H	2.36847900	-0.80767000	1.93249200
H	4.46421500	-1.48518500	0.92974500
H	-0.07620700	-2.36907100	-0.96019700
H	3.66891700	0.31419600	2.28073000
H	2.19728300	-3.11358400	-1.45132500
H	4.64659500	0.03037800	0.07790000
H	4.11777500	-1.90694700	-1.32214000
H	3.06086800	-0.55761800	-1.60043200

C	1.26527600	0.62917600	-0.13202700
C	2.10165900	1.12124700	1.02443900
H	2.70529700	1.98494900	0.72476300
H	1.47169600	1.43119100	1.86827600
H	0.33589100	-0.89312000	1.00839400
H	1.59462500	0.90152300	-1.13432500
N	-1.65234500	0.92820700	0.95877800
S	-2.46786400	-1.44714400	-0.10662200
O	-1.81616900	-2.21567200	1.00876900
C	-4.03843200	-0.81979300	0.55035100
H	-4.68238000	-1.68673100	0.70768700
H	-3.83149800	-0.31516400	1.49560300
H	-4.48702500	-0.13684200	-0.17514900
C	0.47180100	3.53769300	-0.35799800
H	1.21439700	3.43510100	-1.15185500
H	-0.14609200	4.41301000	-0.58094000
H	0.96628800	3.69689300	0.60109800

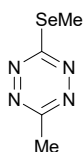


C	0.51993500	0.38259800	-0.00003700
C	-1.97076500	-0.15759800	0.00003100
N	-1.60272900	1.13405600	0.00010600
N	-1.10934400	-1.18256500	0.00003200
N	-0.32819600	1.41852800	0.00006000
N	0.17078900	-0.90879200	-0.00002600
N	1.86245700	0.69827700	-0.00020300
C	2.83569000	-0.03868000	-0.00001700
O	3.84436600	-0.61120900	0.00010700
C	-3.43493100	-0.46037000	-0.00003100
H	-3.90835600	-0.02230300	-0.88258000
H	-3.58823900	-1.53936000	0.00069400
H	-3.90874400	-0.02089800	0.88157400



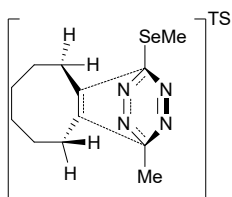
C	-1.88683900	0.02345000	-0.30911500
C	-0.66210500	2.18852700	-0.19505100
N	-1.11278000	1.79955700	-1.42648700
N	-1.34160900	1.81409600	0.92817500
N	-1.74534200	0.68338600	-1.49136900
C	0.30865600	-0.55878100	-0.04850500

C	0.52929200	-1.56127200	-1.14128300
C	2.69818300	-0.12830500	1.54806000
C	1.89738200	-2.23123700	-0.85125300
C	3.63862100	-0.69354400	0.46812100
C	3.09594000	-1.25687200	-0.87007700
H	0.56607200	-1.05880900	-2.11544400
H	1.84551200	-2.75087100	0.11496100
H	2.06239200	-0.93775400	1.92573500
H	4.20709500	-1.49627500	0.95474300
H	-0.26203900	-2.31562200	-1.17970900
H	3.32149800	0.18496000	2.39450700
H	2.05517700	-3.00926400	-1.60613900
H	4.37820900	0.07682100	0.21228900
H	3.94474100	-1.77567000	-1.33012800
H	2.86613000	-0.43385700	-1.55592400
C	0.98644300	0.63199000	-0.07034700
C	1.78086100	1.04664200	1.14593200
H	2.37492600	1.94109100	0.93000100
H	1.11738500	1.28397300	1.98746700
H	0.08386600	-0.98300000	0.93310000
H	1.35672800	0.96895400	-1.03761000
N	-1.97973700	0.70011900	0.87144600
N	-2.48019700	-1.23013800	-0.37933500
C	-2.95849300	-1.91903500	0.50348800
O	-3.44043900	-2.68262500	1.23704200
C	0.12180900	3.46377700	-0.12910000
H	-0.53841900	4.31058500	-0.33911800
H	0.54448000	3.59301400	0.86828900
H	0.91889200	3.46154400	-0.87559200

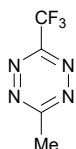


C	-0.03403000	-0.16301400	-0.00004600
C	2.50780700	0.09635800	-0.00004800
N	1.76872800	1.20574500	-0.00008900
N	2.00029600	-1.15312700	-0.00013600
N	0.45778000	1.07391100	-0.00003700
N	0.70659900	-1.28901400	-0.00016400
Se	-1.89626800	-0.42922900	0.00007200
C	-2.40913500	1.44426800	-0.00006400
H	-2.02137600	1.92682800	0.89460400
H	-2.02067100	1.92679800	-0.89444700
H	-3.49924300	1.45555000	-0.00052400
C	3.99721600	0.23097700	0.00017200
H	4.41915900	-0.25751900	0.88249800

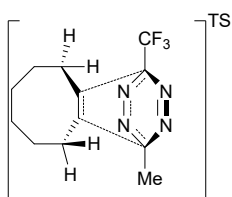
H	4.41955300	-0.25806200	-0.88164500
H	4.27071500	1.28605600	-0.00002400



C	1.40896700	0.59707900	-0.15180200
C	-0.29029100	2.34561900	0.38801600
N	0.49649800	1.91797000	1.41983700
N	0.20907900	2.35199600	-0.88894900
N	1.36921800	1.01248400	1.14455000
C	-0.60953700	-0.47606800	-0.18486900
C	-0.40061900	-1.69235800	0.66501400
C	-3.31567600	-0.38985200	-1.25173400
C	-1.62865200	-2.61254900	0.45046000
C	-3.88497100	-1.34726600	-0.19024200
C	-2.97379400	-1.99094300	0.88458400
H	-0.33658900	-1.41162400	1.72432500
H	-1.67070900	-2.91034400	-0.60575500
H	-2.60905000	-0.93926600	-1.88492300
H	-4.36427300	-2.16386500	-0.74515900
H	0.51524000	-2.21937900	0.37982800
H	-4.14441500	-0.09729300	-1.90823500
H	-1.45850900	-3.53388600	1.01849600
H	-4.69805000	-0.83580600	0.34205600
H	-3.57909300	-2.78018700	1.34523900
H	-2.78461500	-1.27484500	1.69189000
C	-1.50892300	0.48432300	0.20870400
C	-2.60978600	0.88594800	-0.74771000
H	-3.32709500	1.54790200	-0.25057700
H	-2.19996400	1.42819100	-1.60943900
H	-0.49647200	-0.64543800	-1.25803800
H	-1.74593500	0.52714900	1.27097300
N	1.07818600	1.45225400	-1.16981900
Se	2.61504000	-0.78505000	-0.63298600
C	3.24004100	-1.20875000	1.15816700
H	3.79877500	-0.36187700	1.55027900
H	2.39805100	-1.44071900	1.80901800
H	3.88839000	-2.07873700	1.04909400
C	-1.33034300	3.37478200	0.71541600
H	-0.84145400	4.31231000	0.99648300
H	-1.96143100	3.56091600	-0.15474100
H	-1.94352800	3.04577800	1.55736200

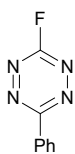


C	-0.30578800	0.03344900	-0.00006000
C	2.22950300	0.00675600	-0.00002400
N	1.61903000	1.19662800	-0.00008400
N	1.58993400	-1.17960700	-0.00007800
N	0.30283200	1.21002000	-0.00005100
N	0.28564000	-1.16426400	-0.00008400
C	-1.82357600	0.00518200	-0.00002300
F	-2.26798000	-0.64091300	1.07952000
F	-2.33062300	1.23163100	-0.00004500
F	-2.26816800	-0.64108600	-1.07929000
C	3.72286200	-0.02270700	0.00009700
H	4.08386200	-0.55762500	0.88247900
H	4.08399200	-0.55923300	-0.88124400
H	4.11302300	0.99464600	-0.00075500

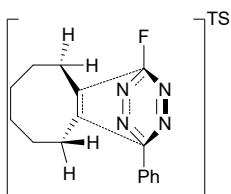


C	-1.70895600	0.20934400	0.00665400
C	-0.40510800	2.28964800	-0.35419400
N	-1.00761100	1.74907300	-1.45066800
N	-0.94004900	2.11547900	0.88852400
N	-1.68398400	0.66713500	-1.26516100
C	0.52129600	-0.52364100	0.13424300
C	0.58625200	-1.71261300	-0.78063800
C	3.09627100	0.07112900	1.34475700
C	1.97527000	-2.36374600	-0.54567300
C	3.89103300	-0.69777500	0.27435100
C	3.17746200	-1.45268300	-0.87559800
H	0.49761900	-1.39748400	-1.82745700
H	2.03492400	-2.70860400	0.49522900
H	2.49345400	-0.64032400	1.92134500
H	4.50036500	-1.43028600	0.81881200
H	-0.19745300	-2.44500100	-0.57799100
H	3.81995400	0.49652300	2.05077100
H	2.02605200	-3.26506000	-1.16625400
H	4.60700000	-0.00780200	-0.19179600
H	3.95244900	-2.07315400	-1.33999500
H	2.87833200	-0.74643500	-1.65802800
C	1.22116000	0.60972000	-0.17440600
C	2.15909700	1.19579600	0.85445400

H	2.74025900	2.01730000	0.42207800
H	1.60490500	1.59608000	1.71329300
H	0.39016100	-0.75682200	1.19233900
H	1.47027200	0.77154800	-1.22242300
N	-1.61683500	1.03554700	1.07499000
C	-2.46790600	-1.07708100	0.25377500
F	-3.73204900	-0.82361200	0.59764300
F	-2.48074600	-1.84557300	-0.83530100
F	-1.91068000	-1.77611700	1.25102000
C	0.46037700	3.49080000	-0.57083000
H	-0.16868100	4.34539100	-0.83828200
H	1.00354200	3.73279500	0.34348000
H	1.15998700	3.31502000	-1.39054400

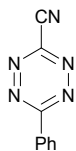


C	-2.91026700	-0.00002200	0.00019500
C	-0.38154400	-0.00003600	-0.00019300
N	-1.01630900	1.18455200	-0.00003100
N	-2.32435400	1.18703600	0.00011200
N	-1.01629600	-1.18456300	-0.00009100
N	-2.32439500	-1.18703800	-0.00002000
C	1.09510100	-0.00000700	-0.00009100
C	1.79531000	-1.21096400	-0.00000500
C	1.79528400	1.21095700	-0.00008000
C	3.18483000	-1.20650200	0.00008000
H	1.24417500	-2.14461000	-0.00000700
C	3.18481100	1.20651900	0.00001200
H	1.24414400	2.14460000	-0.00014700
C	3.88165300	0.00001800	0.00009100
H	3.72498100	-2.14772600	0.00014300
H	3.72493800	2.14775700	0.00001800
H	4.96724700	0.00002400	0.00016200
F	-4.22300900	0.00003100	0.00000000



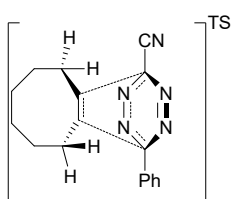
C	-1.21384500	-2.34217800	-0.16929400
C	0.98224200	-1.23212800	0.02135200
N	0.48158300	-1.80312600	1.15713200
N	0.66101700	-1.74863600	-1.20031500
N	-0.65479400	-2.39974600	1.05809200

C	-1.78494200	-0.19789500	-0.22229900
C	-2.89796000	-0.13778100	0.78484700
C	-1.23468700	2.40334800	-1.41113800
C	-3.55494200	1.25667700	0.62461900
C	-1.92131400	3.17449300	-0.26896000
C	-2.60352800	2.43951500	0.91315900
H	-2.49838500	-0.24078100	1.80101400
H	-3.97179600	1.34242600	-0.38781400
H	-1.99236100	1.82892900	-1.95724000
H	-2.68221900	3.80548000	-0.74578400
H	-3.63734100	-0.92793400	0.62848600
H	-0.84718500	3.14406500	-2.12116700
H	-4.40849100	1.30628700	1.30957700
H	-1.19323400	3.87051600	0.16818400
H	-3.17574500	3.21108300	1.44107200
H	-1.84635000	2.11105000	1.63398800
C	-0.62195200	0.48532400	0.01171500
C	-0.09160000	1.43726700	-1.02797400
H	0.77625700	1.98180300	-0.64239600
H	0.23327900	0.89753100	-1.92765100
H	-2.11294600	-0.27450000	-1.26151500
H	-0.35872500	0.68887500	1.04899100
N	-0.47460500	-2.34625900	-1.29937600
C	2.21142400	-0.41916200	0.13332800
C	2.94693500	-0.09173400	-1.00961600
C	2.61341500	0.06657100	1.38121900
C	4.07522900	0.71400000	-0.90084200
H	2.63039600	-0.47866100	-1.97227400
C	3.74177500	0.87207300	1.48245200
H	2.04022300	-0.19974500	2.26347600
C	4.47402000	1.19904800	0.34262600
H	4.64552200	0.96249200	-1.79034200
H	4.05121100	1.24497400	2.45374200
H	5.35419600	1.82923200	0.42400600
F	-2.42448100	-2.86481900	-0.27625100



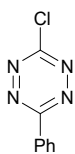
C	2.63879000	-0.00003900	0.00011000
C	0.09152900	-0.00004200	-0.00041300
N	0.72670400	1.18801500	-0.00026600
N	2.03046900	1.19193800	-0.00010200
N	0.72668000	-1.18804300	-0.00012800
N	2.03049800	-1.19196200	0.00007300

C	-1.37975800	-0.00000600	-0.00017500
C	-2.07920200	-1.21292700	-0.00012500
C	-2.07916600	1.21292500	-0.00000200
C	-3.46803100	-1.20784800	0.00008800
H	-1.52746200	-2.14614000	-0.00026100
C	-3.46800300	1.20788200	0.00020000
H	-1.52741500	2.14613100	-0.00003900
C	-4.16345800	0.00002900	0.00024800
H	-4.00934400	-2.14820400	0.00012400
H	-4.00928200	2.14825800	0.00032400
H	-5.24903800	0.00003900	0.00041000
C	4.08326400	0.00000600	0.00018000
N	5.23804000	0.00005700	0.00024800

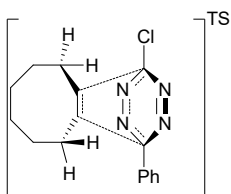


C	-1.47592800	-2.09156800	-0.10314300
C	0.87879600	-1.30944200	0.05182700
N	0.31117100	-1.78514400	1.20440600
N	0.47705900	-1.80916200	-1.15701500
N	-0.90351700	-2.19050300	1.13175000
C	-1.68688900	0.19725500	-0.18673800
C	-2.72988500	0.50455500	0.84738600
C	-0.67011400	2.60180200	-1.46834900
C	-3.09564000	2.00091600	0.66177200
C	-1.14790600	3.52899900	-0.33644900
C	-1.92090100	2.97790000	0.88829100
H	-2.32527500	0.34864800	1.85484500
H	-3.52186800	2.14329600	-0.34009900
H	-1.54513300	2.17476500	-1.97276200
H	-1.78451400	4.28500500	-0.81331100
H	-3.62543700	-0.11348300	0.73592100
H	-0.16684500	3.22723300	-2.21552000
H	-3.89931000	2.23349100	1.36855000
H	-0.28075200	4.07746400	0.05432200
H	-2.31271700	3.86115200	1.40545000
H	-1.22031300	2.52582900	1.59935600
C	-0.39974500	0.63225200	0.00072200
C	0.27158500	1.44081300	-1.08111800
H	1.23738400	1.81754500	-0.72948300
H	0.46301400	0.82637100	-1.97099000
H	-2.05079200	0.14543200	-1.21542300
H	-0.08493000	0.82338800	1.02569700
N	-0.73673400	-2.21306100	-1.24438200

C	2.21857200	-0.69667100	0.13976100
C	2.99505300	-0.53259200	-1.01160500
C	2.69301300	-0.23805300	1.37290400
C	4.23653200	0.08792400	-0.92566600
H	2.62079000	-0.89992000	-1.96111800
C	3.93378600	0.38290900	1.45041000
H	2.08665000	-0.38093300	2.26167000
C	4.70659300	0.54885400	0.30213600
H	4.83917700	0.21039400	-1.81994800
H	4.30000400	0.73659300	2.40891900
H	5.67524900	1.03477200	0.36528500
C	-2.87443100	-2.44095500	-0.20313900
N	-4.00502400	-2.66590500	-0.28266700

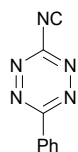


C	-2.50612000	-0.00004000	0.00008700
C	0.03764400	-0.00004800	0.00022500
N	-0.59744200	1.18437000	0.00018100
N	-1.90456100	1.18815200	0.00012900
N	-0.59741600	-1.18439900	0.00011200
N	-1.90460100	-1.18817000	0.00001700
C	1.51276000	-0.00000900	0.00008700
C	2.21277800	-1.21145100	0.00006000
C	2.21273800	1.21144500	-0.00001200
C	3.60212100	-1.20687000	-0.00006700
H	1.66117000	-2.14481000	0.00014000
C	3.60209100	1.20690300	-0.00012900
H	1.66111900	2.14479600	0.00001000
C	4.29856500	0.00003000	-0.00015900
H	4.14264000	-2.14784000	-0.00008800
H	4.14257200	2.14789400	-0.00020200
H	5.38416200	0.00004000	-0.00025400
Cl	-4.22346900	0.00002900	-0.00019000



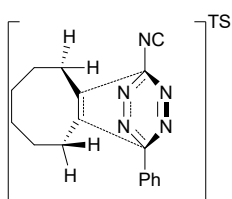
C	-1.53492900	-1.93871600	-0.09477400
C	0.85136800	-1.26617400	0.05594700
N	0.26196800	-1.71158500	1.20779900
N	0.42298400	-1.74237000	-1.15159300
N	-0.96941900	-2.07177000	1.13308300

C	-1.61576700	0.33466000	-0.15517400
C	-2.60043000	0.71257800	0.91242200
C	-0.52740800	2.67635100	-1.50515500
C	-2.90439700	2.22088700	0.71563100
C	-0.92274600	3.64167300	-0.37319500
C	-1.68025000	3.14745400	0.88524600
H	-2.16319700	0.55323200	1.90570900
H	-3.35771200	2.36820400	-0.27375800
H	-1.43815000	2.28480000	-1.97383200
H	-1.53771000	4.42087500	-0.84127700
H	-3.52684200	0.13549700	0.85071600
H	-0.02002300	3.26658700	-2.27791500
H	-3.67133600	2.50248900	1.44542800
H	-0.01770800	4.15302000	-0.01964800
H	-2.01522800	4.05695800	1.39711300
H	-0.97823700	2.67710900	1.58268900
C	-0.30692300	0.71997300	-0.01488900
C	0.36922500	1.47652900	-1.13003300
H	1.36349900	1.81037700	-0.81648100
H	0.49959400	0.83963300	-2.01499800
H	-2.01918300	0.29441000	-1.16931300
H	0.04567000	0.91948800	0.99597200
N	-0.80816700	-2.09802500	-1.23267500
C	2.22893500	-0.73687400	0.14391900
C	3.01484400	-0.61942500	-1.00636600
C	2.73207500	-0.31058000	1.37676300
C	4.29339100	-0.07911900	-0.91960600
H	2.61773800	-0.95957800	-1.95672300
C	4.01025200	0.22977400	1.45585700
H	2.11758600	-0.41574700	2.26521900
C	4.79272900	0.34839300	0.30863400
H	4.90203500	0.00673900	-1.81421500
H	4.39742600	0.55795000	2.41530600
H	5.79040900	0.77149700	0.37248000
Cl	-3.20823600	-2.36597600	-0.21765500



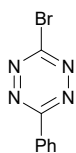
C	-2.65816200	0.00027000	-0.00070900
C	-0.11350700	0.00026200	0.00445500
N	-0.74960800	1.18589800	-0.00025400
N	-2.05396900	1.19152600	-0.00078200
N	-0.74966300	-1.18551600	-0.00019500
N	-2.05381700	-1.19112500	-0.00074100
N	-4.03102800	-0.00013900	-0.00019600

C	-5.20911200	-0.00062700	-0.00086600
C	1.35982600	0.00009200	0.00190300
C	2.05938100	-1.21216600	0.00083900
C	2.05969100	1.21217800	0.00086900
C	3.44853700	-1.20750500	-0.00089100
H	1.50774800	-2.14552100	0.00143400
C	3.44883500	1.20715200	-0.00085000
H	1.50826400	2.14565700	0.00149900
C	4.14471100	-0.00027600	-0.00169100
H	3.98923900	-2.14832900	-0.00158500
H	3.98980600	2.14782000	-0.00150500
H	5.23033800	-0.00040300	-0.00302200

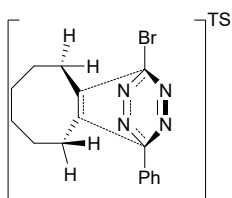


C	-1.45359700	-2.10435300	-0.11359200
C	0.88446100	-1.28368800	0.04563700
N	0.32363000	-1.77448300	1.19439200
N	0.48898600	-1.78037200	-1.16577100
N	-0.88167700	-2.20703500	1.11879900
C	-1.69120400	0.16105500	-0.18497900
C	-2.74265700	0.44379900	0.84676000
C	-0.73060100	2.59283200	-1.46235400
C	-3.14706000	1.92989900	0.66099700
C	-1.23537000	3.50678500	-0.33133000
C	-1.99739700	2.93550700	0.89098100
H	-2.33701300	0.29805400	1.85530000
H	-3.57371600	2.06208000	-0.34214500
H	-1.59301400	2.14459500	-1.97004700
H	-1.88975700	4.24662300	-0.80957200
H	-3.62160100	-0.19746100	0.73324200
H	-0.24073100	3.23156900	-2.20720100
H	-3.95817600	2.14233700	1.36571300
H	-0.38370200	4.07702600	0.06234800
H	-2.41172800	3.80835400	1.40831800
H	-1.28740000	2.49968400	1.60288100
C	-0.41608400	0.62898000	0.00513000
C	0.23832900	1.45507200	-1.07356400
H	1.19411200	1.85438200	-0.71952100
H	0.44642400	0.84630200	-1.96355500
H	-2.05327900	0.10436400	-1.21407900
H	-0.10645100	0.82471100	1.03083400
N	-0.71559300	-2.21134100	-1.25434400
C	2.21985400	-0.65925300	0.13805200

C	2.99551300	-0.48005500	-1.01141000
C	2.68972000	-0.20359700	1.37384100
C	4.23125400	0.15140900	-0.92096100
H	2.62521800	-0.84443200	-1.96361700
C	3.92491800	0.42816600	1.45615100
H	2.08423700	-0.35734500	2.26139500
C	4.69699200	0.60871800	0.30977200
H	4.83284300	0.28526000	-1.81437900
H	4.28702700	0.77913500	2.41726800
H	5.66106600	1.10321200	0.37652700
N	-2.77840000	-2.47473700	-0.20918800
C	-3.92256800	-2.74005600	-0.27861700

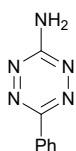


C	1.80540400	-0.00001200	-0.00003600
C	-0.73904900	-0.00000400	-0.00009900
N	-0.10438800	-1.18464400	-0.00014500
N	-0.10436300	1.18464900	-0.00013000
N	1.20320000	-1.18797800	-0.00010700
N	1.20320200	1.18797900	-0.00009300
C	-2.21409800	0.00000600	-0.00003000
C	-2.91412400	1.21145800	-0.00000300
C	-2.91411900	-1.21145000	0.00000600
C	-4.30345900	1.20690600	0.00006300
H	-2.36244600	2.14476200	-0.00003500
C	-4.30345200	-1.20690900	0.00007500
H	-2.36243300	-2.14475000	-0.00002000
C	-4.99989800	-0.00000300	0.00010200
H	-4.84399300	2.14785900	0.00008400
H	-4.84398200	-2.14786500	0.00010600
H	-6.08549100	-0.00000700	0.00015500
Br	3.67461600	0.00000000	0.00007300



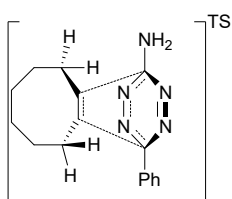
C	-1.56327600	-1.34742400	-0.02956700
C	0.91607700	-1.28828400	0.08315000
N	0.25227400	-1.56138700	1.24812600
N	0.36532300	-1.65691600	-1.11249500
N	-1.03166700	-1.60462300	1.19330900
C	-1.08454100	0.87521500	-0.11757900

C	-1.91748600	1.50054100	0.96267900
C	0.52123000	2.85379900	-1.53050400
C	-1.84280000	3.03367700	0.74316200
C	0.40357100	3.90289100	-0.41010000
C	-0.42387500	3.63057100	0.87170000
H	-1.50808000	1.25089500	1.94927400
H	-2.26862400	3.27517800	-0.23995800
H	-0.46856500	2.69427000	-1.97461900
H	-0.00944100	4.80365900	-0.88179600
H	-2.95782600	1.16738800	0.93013700
H	1.14148200	3.28880400	-2.32364800
H	-2.49896300	3.50664900	1.48199200
H	1.41499300	4.17846800	-0.08349100
H	-0.51161500	4.60220400	1.37135600
H	0.15559000	3.01123800	1.56535700
C	0.28181200	0.92475200	-0.00870800
C	1.10007600	1.47393500	-1.14947500
H	2.15270000	1.55450400	-0.85982600
H	1.04883900	0.81292400	-2.02483800
H	-1.51123500	0.92302800	-1.12186500
H	0.69480500	1.04466600	0.99179400
N	-0.91701800	-1.69385900	-1.17442600
C	2.38272600	-1.11514900	0.14656600
C	3.15457400	-1.20789800	-1.01547900
C	2.99588100	-0.81688800	1.36712800
C	4.52874100	-1.00344300	-0.95257800
H	2.66998600	-1.44689800	-1.95600700
C	4.36964500	-0.61230400	1.42233800
H	2.38876000	-0.75745800	2.26483100
C	5.13854700	-0.70354300	0.26351000
H	5.12520800	-1.08051800	-1.85614700
H	4.84182300	-0.38285400	2.37234900
H	6.21121300	-0.54295500	0.30902400
Br	-3.44453800	-1.33966800	-0.13922800



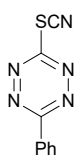
C	-2.92580600	0.00001800	-0.01062900
C	-0.36404900	0.00005800	0.01372900
N	-1.00090700	-1.18158800	0.02812700
N	-1.00087900	1.18168900	0.02524700
N	-2.30327200	-1.19389400	0.01841400
N	-2.30328400	1.19395300	0.01575200
C	1.11487600	0.00002400	0.00491000
C	1.81773300	1.20907200	0.00089100

C	1.81765000	-1.20906700	-0.00123700
C	3.20767700	1.20516200	-0.00871400
H	1.26616900	2.14255600	0.00548200
C	3.20758800	-1.20523500	-0.01085700
H	1.26601700	-2.14251900	0.00180100
C	3.90632700	-0.00005600	-0.01452700
H	3.74700600	2.14718200	-0.01178600
H	3.74685900	-2.14728100	-0.01569300
H	4.99195300	-0.00009800	-0.02222900
N	-4.27749000	-0.00012200	-0.08882900
H	-4.75453200	-0.86760300	0.10576300
H	-4.75463000	0.86763600	0.10429600

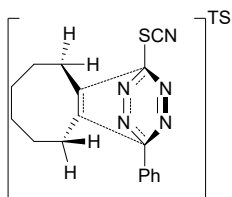


C	-1.33581400	-2.32617400	-0.14720600
C	0.87922300	-1.17325600	0.02769000
N	0.39195200	-1.75574000	1.17520000
N	0.56723100	-1.72831700	-1.18978500
N	-0.73578800	-2.34820900	1.09264500
C	-1.77225800	-0.17636900	-0.22002100
C	-2.87613000	-0.00101000	0.78390800
C	-1.12881100	2.41062400	-1.43238400
C	-3.45838800	1.42342700	0.61664000
C	-1.74054400	3.24162200	-0.29188500
C	-2.44944600	2.55696800	0.90204600
H	-2.48368800	-0.11862400	1.80185400
H	-3.86702500	1.52649200	-0.39766900
H	-1.93094500	1.86880300	-1.94817500
H	-2.46704100	3.91689500	-0.76191400
H	-3.67592700	-0.73712600	0.64239900
H	-0.72022500	3.11444000	-2.16786800
H	-4.31048500	1.52023300	1.29881700
H	-0.95998100	3.89115100	0.12558800
H	-2.97990000	3.35871600	1.42847100
H	-1.70664800	2.19293900	1.62032800
C	-0.56485800	0.45833900	-0.00421200
C	-0.02774800	1.39834200	-1.05811500
H	0.86697400	1.91085300	-0.69036600
H	0.26242300	0.84164500	-1.95888100
H	-2.10798200	-0.23562500	-1.25810000
H	-0.32226300	0.70856900	1.02764900
N	-0.55829800	-2.32320300	-1.28515100
C	2.16587800	-0.44362300	0.13497300

C	2.94118800	-0.20102500	-1.00244100
C	2.58429300	0.05029400	1.37397500
C	4.12194400	0.52704600	-0.89750500
H	2.61337100	-0.59396700	-1.95882800
C	3.76521300	0.77788800	1.47238700
H	1.98257300	-0.15219100	2.25440200
C	4.53645100	1.02018900	0.33746400
H	4.72161400	0.70777000	-1.78431000
H	4.08523800	1.15560000	2.43862200
H	5.45761200	1.58930400	0.41607100
N	-2.54298300	-2.98122500	-0.24417600
H	-3.12466700	-2.91762100	0.58007300
H	-3.02898700	-2.85107700	-1.12117100

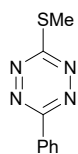


C	-1.91656900	0.46508800	0.00005600
C	0.60885800	0.16166200	-0.00016800
N	-0.16448100	-0.93728900	-0.00079600
N	0.12090000	1.41717300	0.00025600
N	-1.46353000	-0.78488700	-0.00065400
N	-1.17348500	1.57392600	0.00040900
C	2.07227700	-0.01623500	-0.00006900
C	2.91410700	1.10159200	-0.00059200
C	2.61982200	-1.30410700	0.00057200
C	4.29253300	0.92821900	-0.00049500
H	2.48085800	2.09543600	-0.00106000
C	3.99930500	-1.46806200	0.00070200
H	1.95939700	-2.16392600	0.00094200
C	4.83710800	-0.35446200	0.00016600
H	4.94339200	1.79649700	-0.00093900
H	4.42154600	-2.46766000	0.00123800
H	5.91463000	-0.48626600	0.00025800
S	-3.66201100	0.80219500	0.00044600
C	-4.26003400	-0.79129500	-0.00007800
N	-4.76684500	-1.83229400	-0.00037800



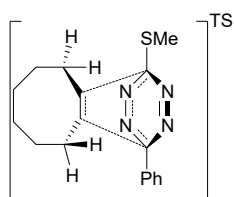
C	1.44907000	-1.67931100	-0.26974900
C	-1.00375400	-1.29662200	-0.15555200
N	-0.48966700	-1.62909200	-1.37862200

N	-0.39786000	-1.75290900	0.98431900
N	0.77897400	-1.82807800	-1.44007500
C	1.27398400	0.61277300	-0.06387100
C	2.14252200	1.15783100	-1.15971400
C	-0.01076800	2.74228900	1.45144500
C	2.25984700	2.68425800	-0.90831000
C	0.18366100	3.79355700	0.34489900
C	0.91909600	3.44753100	-0.97387600
H	1.68095600	0.97893200	-2.13874900
H	2.74556900	2.84702900	0.06274600
H	0.97009400	2.45410700	1.84761400
H	0.72156100	4.62855600	0.81137900
H	3.14142900	0.71249000	-1.16737800
H	-0.53889800	3.23013300	2.27958700
H	2.94329100	3.09083100	-1.66160400
H	-0.80001900	4.19435000	0.06679000
H	1.10273400	4.40938600	-1.46613700
H	0.24247100	2.91260300	-1.64989000
C	-0.07940100	0.82883800	-0.11257500
C	-0.77148800	1.45290300	1.07379200
H	-1.81761200	1.66869200	0.83413000
H	-0.76471400	0.77279300	1.93596100
H	1.73627400	0.58365300	0.92542000
H	-0.52078000	1.01112200	-1.09171600
N	0.86570600	-1.96596100	0.92599400
C	-2.43385600	-0.93468300	-0.08313100
C	-3.10711100	-0.96032300	1.14198900
C	-3.10510300	-0.52311500	-1.23876800
C	-4.44199500	-0.57572600	1.20611000
H	-2.57905600	-1.28774400	2.03107000
C	-4.43845500	-0.13803900	-1.16659300
H	-2.57593400	-0.51641400	-2.18635100
C	-5.10891200	-0.16179000	0.05523300
H	-4.96294300	-0.60061300	2.15792300
H	-4.95642300	0.17995900	-2.06582100
H	-6.15021000	0.14016600	0.10934800
S	3.20247000	-2.00883600	-0.44220100
C	3.73775400	-1.20787600	0.96059100
N	4.15029600	-0.64162100	1.88400900



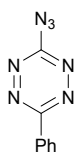
C	-2.14059400	-0.29763100	-0.00004200
C	0.41305500	-0.10227000	0.00016500
N	-0.13306400	-1.33676600	0.00010400

N	-0.30651900	1.02466900	0.00027900
N	-1.42711800	-1.44105500	0.00000200
N	-1.61505800	0.92980400	0.00017400
C	1.88605600	0.00318900	0.00007400
C	2.49855700	1.26099700	-0.00012400
C	2.67291900	-1.15337600	0.00015200
C	3.88462100	1.35719900	-0.00023200
H	1.88042200	2.15177800	-0.00019100
C	4.05881400	-1.04877900	0.00005000
H	2.19006300	-2.12407400	0.00028700
C	4.66743900	0.20435900	-0.00014000
H	4.35543300	2.33510800	-0.00039200
H	4.66533900	-1.94880600	0.00011700
H	5.75023500	0.28271100	-0.00021100
S	-3.87845000	-0.51523800	-0.00029400
C	-4.40999400	1.21830300	0.00016800
H	-5.50076100	1.19187300	0.00001300
H	-4.04934300	1.73309600	0.89062300
H	-4.04910300	1.73361200	-0.88989300

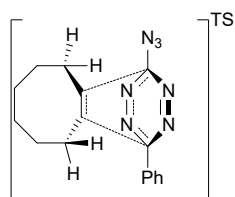


C	1.66296300	-1.54752500	-0.23944400
C	-0.81960800	-1.23944500	-0.18554700
N	-0.25453300	-1.50448500	-1.41204400
N	-0.24164200	-1.75464100	0.94220700
N	1.01238000	-1.66639800	-1.44391100
C	1.34786100	0.66920400	0.00839500
C	2.16386300	1.30239900	-1.08020300
C	-0.01029000	2.69834600	1.61158800
C	2.22244700	2.82150800	-0.77895600
C	0.11760700	3.79509300	0.53965500
C	0.85107800	3.53181100	-0.79933500
H	1.68314900	1.14138900	-2.05318700
H	2.71523900	2.97655500	0.19044800
H	0.99042600	2.44441200	1.98174200
H	0.61997000	4.63961400	1.02858200
H	3.17580300	0.89063700	-1.12799600
H	-0.54504600	3.13415700	2.46444600
H	2.87588600	3.28319800	-1.52742600
H	-0.88855400	4.15572200	0.28829500
H	0.98889800	4.51950000	-1.25429100
H	0.18926000	2.99620200	-1.48887400
C	-0.01957100	0.82818000	-0.01220100

C	-0.71726500	1.38918700	1.20289300
H	-1.77549100	1.56686100	0.98601000
H	-0.66857000	0.68173300	2.04119600
H	1.82514400	0.64436400	0.99053700
H	-0.46899900	1.06090900	-0.97625200
N	1.03101400	-1.91350000	0.91755300
C	-2.27556500	-0.97000600	-0.15152800
C	-2.99050600	-1.09513900	1.04322500
C	-2.93165900	-0.54473500	-1.31033400
C	-4.34865700	-0.79687000	1.07433200
H	-2.47435900	-1.43252800	1.93560600
C	-4.28918800	-0.24698100	-1.27230000
H	-2.37103200	-0.46202700	-2.23608300
C	-5.00070600	-0.37040600	-0.08047700
H	-4.89991500	-0.89973200	2.00385700
H	-4.79367000	0.08043300	-2.17601600
H	-6.06048800	-0.13666100	-0.05259500
S	3.41599600	-1.76659000	-0.33659000
C	3.81369400	-1.82894700	1.43164000
H	4.90094500	-1.90314000	1.48973000
H	3.48502200	-0.92120900	1.94156800
H	3.35092000	-2.69582700	1.90108100

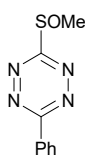


C	-2.25444500	0.47597900	-0.00007200
C	0.27928700	0.16492600	0.00000500
N	-0.49060500	-0.93246100	-0.00038700
N	-0.21394400	1.41907000	0.00038000
N	-1.78774700	-0.77678800	-0.00040700
N	-1.50381800	1.58732700	0.00031300
C	1.74544700	-0.00620000	0.00001400
C	2.58235000	1.11488000	-0.00020400
C	2.30117400	-1.29020100	0.00022900
C	3.96206500	0.94893800	-0.00021200
H	2.14302100	2.10604800	-0.00036200
C	3.68167000	-1.44740700	0.00023400
H	1.64513700	-2.15346300	0.00038200
C	4.51445000	-0.33014800	0.00001300
H	4.60784700	1.82117200	-0.00039500
H	4.10880800	-2.44510100	0.00041700
H	5.59269300	-0.45627300	0.00001100
N	-3.62745900	0.70319300	-0.00017800
N	-4.31920400	-0.33750100	0.00017300
N	-5.05286400	-1.18526700	0.00009300

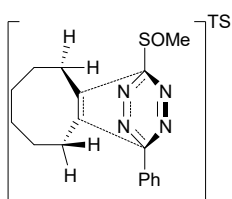


C	-1.60429300	-1.63175100	-0.51239700
C	0.82547200	-1.25990600	-0.11003300
N	0.09818200	-1.75045700	0.94202600
N	0.45177800	-1.57960800	-1.39224900
N	-1.15065500	-1.95111200	0.73633700
C	-1.39910700	0.58306300	-0.39492000
C	-2.49080300	0.98611100	0.55430200
C	0.10271000	2.92435100	-1.28661300
C	-2.59216900	2.53219100	0.51144300
C	-0.33077700	3.80063300	-0.09870900
C	-1.31601300	3.26909800	0.97185200
H	-2.25213000	0.66242800	1.57535500
H	-2.86391700	2.84271200	-0.50616400
H	-0.77506300	2.70292800	-1.90562400
H	-0.77615400	4.70409900	-0.53434800
H	-3.45753700	0.55702000	0.27213300
H	0.76978500	3.52787400	-1.91405900
H	-3.42991200	2.82724500	1.15267500
H	0.56826500	4.14064700	0.43193600
H	-1.62366800	4.14870200	1.54876000
H	-0.78376100	2.63594900	1.69026800
C	-0.08592400	0.79327700	-0.04129900
C	0.80686100	1.59088500	-0.96023400
H	1.78014700	1.76460600	-0.49030800
H	0.98714900	1.04662000	-1.89670500
H	-1.64999600	0.69027400	-1.45223000
H	0.13618700	0.85220200	1.02338300
N	-0.79273100	-1.77910900	-1.60528600
C	2.24935400	-0.93747900	0.13195200
C	3.14290000	-0.83351300	-0.93796500
C	2.69356800	-0.68816600	1.43390200
C	4.46840100	-0.48328700	-0.70323900
H	2.79069300	-1.03612000	-1.94364700
C	4.01939200	-0.33762600	1.66133600
H	1.99493200	-0.78153700	2.25935300
C	4.90936200	-0.23237000	0.59399700
H	5.15955300	-0.40812800	-1.53688000
H	4.35954900	-0.14743700	2.67446400
H	5.94407500	0.04246100	0.77372000
N	-2.97341700	-1.78221200	-0.79287800
N	-3.67808000	-1.99792800	0.21043400

N -4.42247800 -2.19180300 1.02985500

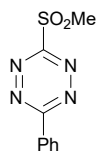


C 1.82383100 -0.00354900 0.21341900
 C -0.71711900 -0.00381600 0.09759300
 N -0.09474300 1.17812800 0.27301600
 N -0.07668800 -1.18079000 -0.00237500
 N 1.20964500 1.17302300 0.33698700
 N 1.23292700 -1.18300700 0.05951700
 C -2.19012200 -0.00581900 0.01696300
 C -2.87810100 -1.21037100 -0.16691800
 C -2.90010800 1.19517800 0.12377600
 C -4.26526900 -1.20911900 -0.24312800
 H -2.31834100 -2.13531000 -0.24794400
 C -4.28727900 1.18737800 0.04649500
 H -2.35828300 2.12327700 0.26674800
 C -4.97162600 -0.01255200 -0.13678100
 H -4.79644600 -2.14459100 -0.38558400
 H -4.83561300 2.12011300 0.12997500
 H -6.05556000 -0.01523900 -0.19657400
 S 3.64390900 0.00814700 0.38345500
 O 4.14807600 -1.33206600 -0.03450900
 C 3.90042500 1.15674800 -1.00285100
 H 4.97171100 1.35992300 -1.04461800
 H 3.57853400 0.66647300 -1.92409800
 H 3.34106200 2.07557900 -0.81854100



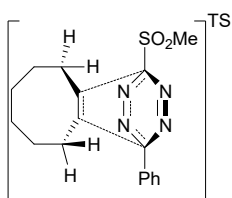
C -1.60392600 -1.29773100 0.17422800
 C 0.88161500 -1.34308000 0.16454700
 N 0.27097700 -1.56288500 1.36362600
 N 0.25842500 -1.70491700 -0.99670700
 N -1.01957100 -1.54169600 1.36811900
 C -1.10214200 0.94969000 -0.03238900
 C -1.90351900 1.63348700 1.03850200
 C 0.52684100 2.81214700 -1.55921200
 C -1.77649600 3.15491100 0.75869400
 C 0.46897100 3.90479900 -0.47631700
 C -0.33531200 3.70507600 0.83350700
 H -1.50196300 1.40497000 2.03336600

H	-2.21674900	3.36868700	-0.22384300
H	-0.47823900	2.66542200	-1.97161300
H	0.07175300	4.80021500	-0.97122800
H	-2.96045000	1.35654900	1.00947000
H	1.14024900	3.19745100	-2.38297400
H	-2.39997700	3.67922200	1.49120900
H	1.49604500	4.16056500	-0.18360700
H	-0.37797400	4.69591400	1.30058900
H	0.24027700	3.09045100	1.53460400
C	0.26353700	0.95980800	0.04558700
C	1.07130300	1.42984800	-1.13669400
H	2.13358400	1.48648900	-0.87750000
H	0.97463800	0.73719500	-1.98356300
H	-1.56551100	0.95002200	-1.02078100
H	0.71129700	1.08511700	1.03094800
N	-1.02683400	-1.68576500	-0.99076400
C	2.34814700	-1.17939900	0.14689100
C	3.05785800	-1.30525100	-1.05133100
C	3.02493600	-0.85489700	1.32677600
C	4.43431200	-1.10764100	-1.06459500
H	2.52357400	-1.56227300	-1.95963600
C	4.40030400	-0.65693000	1.30561900
H	2.46447100	-0.76699600	2.25203100
C	5.10735700	-0.78147700	0.11074800
H	4.98287900	-1.20928100	-1.99563200
H	4.92235200	-0.40534700	2.22336400
H	6.18157500	-0.62540600	0.09652100
S	-3.42335700	-1.15635400	0.20098300
O	-3.81462000	-0.22391500	-0.91089900
C	-3.71360000	-2.83964800	-0.41089600
H	-4.79449400	-2.95884600	-0.50323800
H	-3.22950900	-2.93368300	-1.38441100
H	-3.30924700	-3.55889100	0.30548900



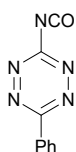
C	-1.55092700	0.08163700	0.00760700
C	0.98639000	0.02361600	0.01284100
N	0.37663300	1.22617800	0.04686800
N	0.33042900	-1.15047200	-0.01056300
N	-0.92864400	1.25653500	0.05378400
N	-0.97778400	-1.11514800	-0.02559500
C	2.45898900	-0.00305100	0.00749000
C	3.13713600	-1.22655600	-0.04294000
C	3.17955600	1.19613600	0.05097400

C	4.52592400	-1.24598600	-0.04939900
H	2.56955000	-2.14955900	-0.07774800
C	4.56831800	1.16697000	0.04436000
H	2.64446000	2.13814400	0.08941200
C	5.24270900	-0.05152400	-0.00567700
H	5.05036700	-2.19504900	-0.08950500
H	5.12570700	2.09727100	0.07826100
H	6.32810000	-0.07038800	-0.01110500
S	-3.36219500	0.12812400	-0.09260300
O	-3.70499300	-0.03608600	-1.49719800
C	-3.82490900	-1.35583500	0.78284700
H	-4.91412300	-1.39847900	0.71612600
H	-3.36929000	-2.21732300	0.29634900
H	-3.50959900	-1.26802900	1.82319900
O	-3.80420700	1.28375300	0.66676900

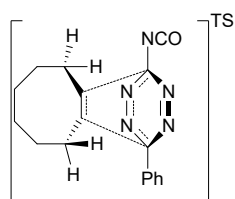


C	-1.52199100	-1.15912600	0.04059900
C	0.94653300	-1.38451500	0.11942300
N	0.27456300	-1.56282000	1.29360300
N	0.34440700	-1.68986500	-1.06615400
N	-1.01029300	-1.45564300	1.25329500
C	-0.85292500	1.09478300	-0.11007800
C	-1.63580100	1.81653900	0.94958100
C	0.97953500	2.83571000	-1.54554800
C	-1.37399200	3.32688900	0.70179200
C	0.96847000	3.91107900	-0.44379100
C	0.10410900	3.75531000	0.83353900
H	-1.28110500	1.53759200	1.94918700
H	-1.76188800	3.59566500	-0.28952100
H	-0.01695100	2.78017200	-1.99921400
H	0.66261700	4.84346600	-0.93531700
H	-2.70801600	1.61714700	0.90214900
H	1.65488000	3.18210100	-2.33748600
H	-1.97640700	3.88747900	1.42479000
H	2.00131900	4.07861900	-0.11047200
H	0.12704900	4.73793900	1.31891300
H	0.60264800	3.08298100	1.54079700
C	0.50333200	0.98840900	0.01409600
C	1.39103900	1.40579500	-1.12977100
H	2.44373600	1.36952100	-0.83086500
H	1.27005600	0.73690300	-1.99261000
H	-1.27193300	1.14875300	-1.11672300

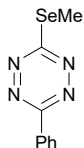
H	0.92428500	1.05128800	1.01704000
N	-0.93754500	-1.57616600	-1.10513700
C	2.41838800	-1.31459600	0.15888600
C	3.16247200	-1.46848500	-1.01518700
C	3.06889200	-1.04970500	1.36831300
C	4.54778900	-1.35672900	-0.97541300
H	2.64748900	-1.67862500	-1.94639900
C	4.45357500	-0.93723100	1.39967800
H	2.48106500	-0.93987200	2.27399000
C	5.19497600	-1.08887900	0.22894600
H	5.12353700	-1.47932900	-1.88721900
H	4.95591300	-0.73139300	2.33943800
H	6.27650100	-0.99932000	0.25606400
S	-3.31236800	-0.93079400	-0.07464800
O	-3.55404600	-0.02949000	-1.19509500
C	-3.86001300	-2.56691600	-0.53581200
H	-4.94292800	-2.50266900	-0.66043100
H	-3.37359400	-2.83957400	-1.47285800
H	-3.60468700	-3.25574400	0.27070600
O	-3.80844800	-0.61912600	1.25705000



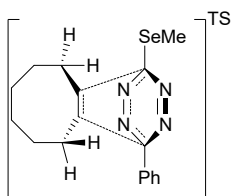
C	-2.20925500	0.42323100	-0.00004200
C	0.33055800	0.14614700	-0.00035100
N	-0.17689400	1.39030100	-0.00013200
N	-0.42781700	-0.96370600	-0.00060100
N	-1.47323500	1.53941000	-0.00000900
N	-1.72362300	-0.82667500	-0.00043400
C	1.79778700	-0.01054200	-0.00016000
C	2.36600400	-1.28909900	0.00003900
C	2.62293300	1.11944300	-0.00009800
C	3.74805300	-1.43212500	0.00028100
H	1.71883600	-2.15898600	0.00000300
C	4.00404900	0.96752100	0.00014000
H	2.17311900	2.10592000	-0.00022200
C	4.56903400	-0.30622800	0.00032300
H	4.18554400	-2.42526700	0.00045000
H	4.64118600	1.84603600	0.00019000
H	5.64850400	-0.42138000	0.00049900
N	-3.57694400	0.59312000	0.00044700
C	-4.46761600	-0.24156600	0.00025900
O	-5.41086100	-0.91677000	0.00022900



C	-1.62341800	-1.60656300	-0.45208200
C	0.82291800	-1.29749300	-0.08143100
N	0.09022800	-1.74213700	0.98773900
N	0.42722100	-1.62348100	-1.35136100
N	-1.16508900	-1.91342200	0.80048000
C	-1.36083900	0.62623300	-0.35264700
C	-2.40179500	1.06974200	0.63319300
C	0.18101600	2.89716400	-1.34198200
C	-2.46653200	2.61740200	0.56107400
C	-0.19358700	3.81008700	-0.16130200
C	-1.15460300	3.33009700	0.95517900
H	-2.12340600	0.76149500	1.64873700
H	-2.77099500	2.91447400	-0.45127900
H	-0.71986900	2.68828300	-1.93133800
H	-0.63102900	4.71396800	-0.60404200
H	-3.39081700	0.65843000	0.40754300
H	0.84636000	3.46870500	-2.00044200
H	-3.26991200	2.94696100	1.22884500
H	0.73020100	4.14021700	0.33176100
H	-1.41792600	4.23141500	1.52041900
H	-0.61354600	2.70027300	1.67002300
C	-0.03312700	0.80276200	-0.04508400
C	0.85611200	1.55024500	-1.00740100
H	1.84736400	1.70477900	-0.56941500
H	0.99233900	0.98082400	-1.93634900
H	-1.64607800	0.72399200	-1.40206800
H	0.22507300	0.87194700	1.01072600
N	-0.82797700	-1.78726800	-1.54717600
C	2.25462100	-0.99953000	0.14210600
C	3.13811800	-0.92882400	-0.93896800
C	2.71781800	-0.74193000	1.43583400
C	4.47300900	-0.60321000	-0.72329300
H	2.77054100	-1.13740700	-1.93791100
C	4.05298300	-0.41573100	1.64401400
H	2.02659500	-0.80964900	2.26994700
C	4.93302400	-0.34383600	0.56571900
H	5.15648700	-0.55386500	-1.56511900
H	4.40822300	-0.21879400	2.65062700
H	5.97512700	-0.08826600	0.73054600
N	-2.98798500	-1.71187100	-0.68204900
C	-3.89981300	-1.89634500	0.10383800
O	-4.86561900	-2.05901800	0.73184400

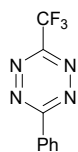


C	-1.54342800	-0.19885200	0.00007100
C	1.01396600	-0.06422700	0.00021400
N	0.44008800	-1.28467800	-0.00010300
N	0.32114100	1.08088300	0.00062600
N	-0.85778200	-1.35697800	-0.00012500
N	-0.98805100	1.01474200	0.00050800
C	2.48878400	0.00778100	0.00009500
C	3.13009000	1.25119700	-0.00049100
C	3.24898100	-1.16648100	0.00051700
C	4.51802000	1.31555000	-0.00064600
H	2.53253900	2.15589500	-0.00084300
C	4.63683800	-1.09380300	0.00037400
H	2.74399900	-2.12584100	0.00093800
C	5.27409300	0.14506700	-0.00020400
H	5.01109600	2.28242200	-0.00112800
H	5.22259400	-2.00747200	0.00071900
H	6.35840700	0.19849900	-0.00031100
Se	-3.41477600	-0.37017200	-0.00032200
C	-3.83463700	1.52633500	0.00056600
H	-3.42397100	1.98964300	-0.89404000
H	-4.92287500	1.59066700	0.00096300
H	-3.42340500	1.98884100	0.89533300



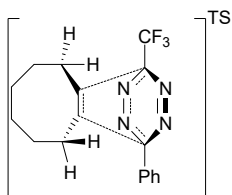
C	-1.48530100	-1.15161600	-0.22490500
C	1.00155300	-1.25559100	-0.00130700
N	0.27050300	-1.56426000	1.11480200
N	0.48385200	-1.53804700	-1.24230200
N	-1.00765100	-1.51203700	1.00216300
C	-0.82417800	0.98750100	-0.22127800
C	-1.71153400	1.65876700	0.78535400
C	1.02603300	2.91422000	-1.39951800
C	-1.50606100	3.18658700	0.63719300
C	0.89157600	3.92843500	-0.25078000
C	-0.07017200	3.66998900	0.93500400
H	-1.43410000	1.35073100	1.80186700
H	-1.80718700	3.49009800	-0.37436700
H	0.06713600	2.84294600	-1.92688200

H	0.59281100	4.87689600	-0.71528800
H	-2.76210900	1.40616500	0.61129800
H	1.73750700	3.33046500	-2.12322200
H	-2.20226500	3.68336900	1.32204100
H	1.88743400	4.10842500	0.17525800
H	-0.13709300	4.62347300	1.47154400
H	0.39269900	2.97848600	1.64779400
C	0.53216200	0.93252900	0.00793900
C	1.47768200	1.48606200	-1.03147400
H	2.50389500	1.48534800	-0.65010500
H	1.46499700	0.86644700	-1.93789300
H	-1.14792700	1.10228600	-1.25834900
H	0.85912100	0.99720800	1.04485600
N	-0.78721400	-1.48688700	-1.36150000
C	2.47493500	-1.21704400	0.13575000
C	3.29529200	-1.33962800	-0.98935400
C	3.04954900	-1.01124400	1.39347200
C	4.67710400	-1.25560100	-0.85341400
H	2.84074900	-1.50735200	-1.95982000
C	4.43108100	-0.92702500	1.52246000
H	2.40462300	-0.92852200	2.26264300
C	5.24816100	-1.04687100	0.39979900
H	5.30982900	-1.35544700	-1.72982300
H	4.87163800	-0.76863300	2.50187700
H	6.32683000	-0.97977600	0.50233900
Se	-3.36311700	-1.02010400	-0.46581900
C	-3.87420300	-1.27029900	1.39281300
H	-3.61870100	-2.28222200	1.69907200
H	-3.36870300	-0.54341400	2.02715800
H	-4.95370000	-1.11983400	1.42720100



C	1.85984700	0.02293500	0.01785000
C	-0.68288300	0.01048900	-0.00068900
N	-0.05559900	1.19901500	0.00308300
N	-0.04344100	-1.17619700	-0.00797400
N	1.25314100	1.20506900	0.01131300
N	1.26057300	-1.16797300	0.00202700
C	-2.15663300	0.00233200	-0.00068500
C	-2.84984800	-1.21341100	0.00363900
C	-2.86225900	1.21097000	-0.00438000
C	-4.23906000	-1.21568600	0.00425000
H	-2.29329500	-2.14373800	0.00664500
C	-4.25127200	1.19916000	-0.00411800

H	-2.31486100	2.14673400	-0.00760800
C	-4.94098000	-0.01185800	0.00028700
H	-4.77523300	-2.15904000	0.00798400
H	-4.79708400	2.13697400	-0.00733000
H	-6.02656000	-0.01735400	0.00074900
C	3.37680100	0.00046600	0.00354800
F	3.81964900	-0.33843800	-1.21055200
F	3.87700200	1.19047200	0.31643900
F	3.83468600	-0.89818400	0.87435900



C	-1.58828500	-1.37945100	-0.02021600
C	0.89329200	-1.32691000	0.08865600
N	0.23311800	-1.59704100	1.25371300
N	0.34044200	-1.68273000	-1.11025800
N	-1.05182600	-1.62762300	1.19869500
C	-1.13816200	0.87787300	-0.16370700
C	-2.04801300	1.51898700	0.84750900
C	0.55728000	2.85946900	-1.47460900
C	-1.93178300	3.05121100	0.63589400
C	0.38968700	3.90381600	-0.35724700
C	-0.51912200	3.62973100	0.86698300
H	-1.73219700	1.26050500	1.86558100
H	-2.28176700	3.29773200	-0.37538800
H	-0.40864200	2.71039600	-1.97197900
H	0.01806700	4.81391600	-0.84510400
H	-3.08964400	1.21568900	0.72758200
H	1.22392400	3.29028000	-2.23155100
H	-2.63499900	3.53224000	1.32455300
H	1.38350300	4.16186600	0.03174300
H	-0.62901600	4.59662700	1.37128100
H	0.00713500	2.99599800	1.58929600
C	0.21794900	0.92651500	0.02633900
C	1.10178300	1.47393300	-1.06604900
H	2.13763900	1.54570800	-0.71921000
H	1.09465900	0.81616100	-1.94552700
H	-1.49590800	0.90839500	-1.19454600
H	0.57745300	1.02949800	1.04942700
N	-0.94154500	-1.71579900	-1.16618300
C	2.35495800	-1.12794000	0.14859100
C	3.12677600	-1.21565200	-1.01395500
C	2.96265900	-0.80775700	1.36662100
C	4.49645600	-0.98254500	-0.95437900

H	2.64577900	-1.47238100	-1.95162100
C	4.33164900	-0.57396300	1.41809900
H	2.35484800	-0.75267500	2.26409400
C	5.10058600	-0.65901800	0.25850100
H	5.09382600	-1.05521300	-1.85765000
H	4.80045800	-0.32636600	2.36516900
H	6.16966600	-0.47543400	0.30129400
C	-3.09921000	-1.40767900	-0.11274700
F	-3.53186800	-2.63041300	-0.42663400
F	-3.65957300	-1.05514500	1.04427700
F	-3.53601500	-0.56936600	-1.06152200