Supplementary Materials

What else than acridinium esters?
Computational search for new acridinium-based chemiluminogens

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Figure S1. The Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) of investigated potential chemiluminogens (R – the central atom in leaving group).

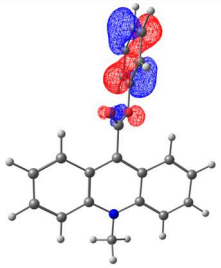
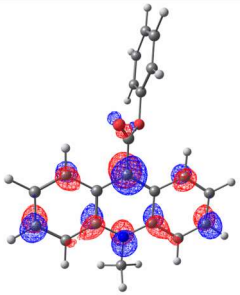
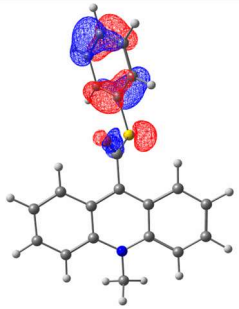
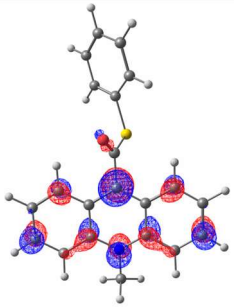
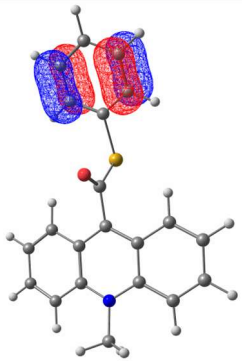
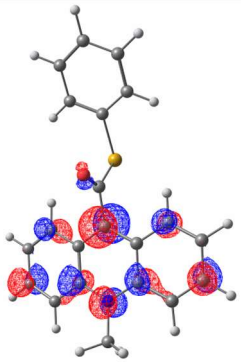
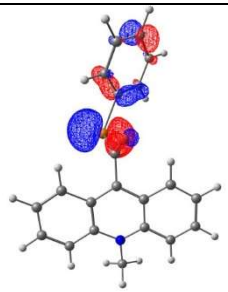
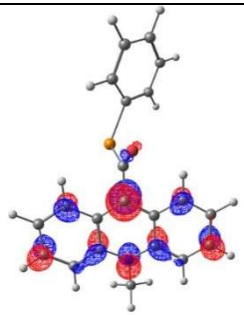
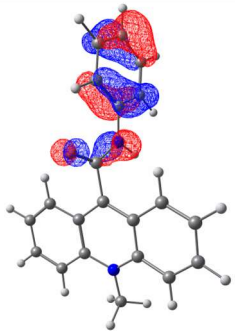
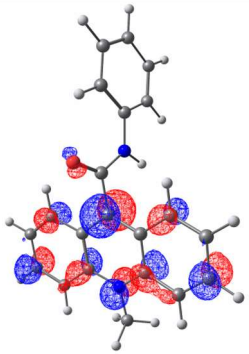
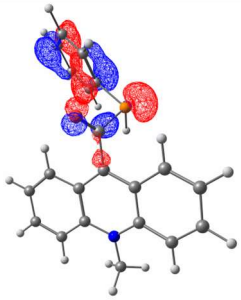
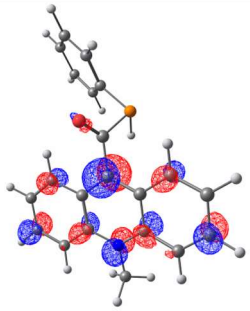
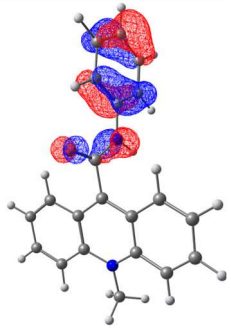
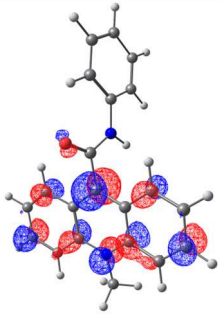
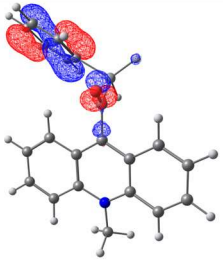
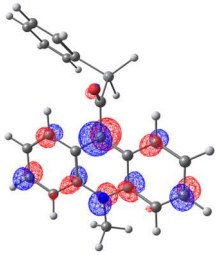
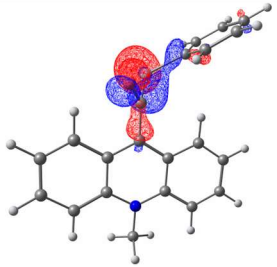
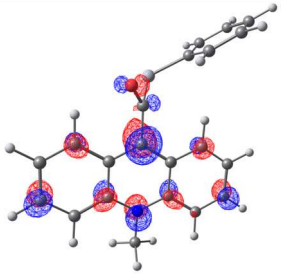
R	orbital		R	orbital		R	orbital	
	HOMO	LUMO		HOMO	LUMO		HOMO	LUMO
O			S			Se		
Te			N (N–H)			P (P–H)		
As (As–H)			Si (H–Si–H)			Ge (H–Ge–H)		

Table S1. The thermodynamic data of the light pathway of chemiluminescence reaction (step I, II, Scheme 1) and the competitive pathways (step IV – formation of the 'pseudobase' and step V – hydrolysis of the acridinium cation, Scheme 1) calculated with different basis sets (LanL2DZ and 6-31G(d,p)) for selected derivatives (R).

Step no. (Scheme 1)	R	Basis set for R	gaseous phase		aqueous phase	Step no. (Scheme 1)	R	Basis set for R	gaseous phase		aqueous phase
			$\Delta_{r,298}H^0$	$\Delta_{r,298}G^0$	$\Delta_{r,298}G^0$				$\Delta_{r,298}H^0$	$\Delta_{r,298}G^0$	$\Delta_{r,298}G^0$
I	Te	LanL2DZ	–165.8	–198.8	–82.7	II	Te	LanL2DZ	–104.1	–117.1	–65.9
	O	6-31G(d,p)	–166.6 [a]	–153.6 [a]	–51.5 [a]		O	6-31G(d,p)	–60.5	–73.7	–47.6
		LanL2DZ	–175.1	–162.3	–54.2			LanL2DZ	–71.1	–85.1	–59.6
	S	6-31G(d,p)	–166.2 [b]	–153.0 [b]	–43.1 [b]		S	6-31G(d,p)	–80.1 [b]	–93.2 [b]	–69.0 [b]
		LanL2DZ	–165.1	–152.1	–42.5			LanL2DZ	–96.2	–108.8	–84.0
	Se	6-31G(d,p)	–166.3	–153.1	–43.8		Se	6-31G(d,p)	–73.1	–86.4	–60.8
		LanL2DZ	–165.2	–153.6	–42.3			LanL2DZ	–94.6	–103.9	–62.8
IV	Te	LanL2DZ	–191.5	–179.2	–103.2	V	Te	LanL2DZ	–115.5	–162.9	–105.4
	O	6-31G(d,p)	–186.1 [a]	–175.6 [a]	–73.3 [a]		O	6-31G(d,p)	–72.5	–74.3	–49.1
		LanL2DZ	–196.2	–186.6	–70.1			LanL2DZ	–92.9	–94.4	–70.6
	S	6-31G(d,p)	–197.1 [b]	–187.5 [b]	–61.9 [b]		S	6-31G(d,p)	–92.0 [b]	–93.2 [b]	–68.9 [b]
		LanL2DZ	–188.9	–187.0	–60.9			LanL2DZ	–107.0	–107.9	–83.3
	Se	6-31G(d,p)	–166.3	–153.1	–43.8		Se	6-31G(d,p)	–73.1	–86.4	–60.8
		LanL2DZ	–191.2	–182.7	–62.8			LanL2DZ	–109.1	–111.5	–86.2

$\Delta_{r,298}H^0$ and $\Delta_{r,298}G^0$ (both in kcal mol^{-1}), respectively, represent the enthalpy and Gibbs' free energy (gaseous phase) or free energy (aqueous phase) of the reaction corresponding to a given step number at standard temperature and pressure;
[a] [1]; [b] [2].

[1] Krzymiński, K.; Ożóg, A.; Malecha, P.; Roshal, A.D.; Wróblewska, A.; Zadykowicz, B.; Błażejowski, J. Chemiluminogenic Features of 10-Methyl-9-(Phenoxycarbonyl)Acridinium Trifluoromethanesulfonates Alkyl Substituted at the Benzene Ring in Aqueous Media. *J. Org. Chem.* **2011**, *76*, 1072–1085. https://doi.org/10.1021/jo1020882.

[2] Pieńkos, M.; Zadykowicz, B. Computational Insights on the Mechanism of the Chemiluminescence Reaction of New Group of Chemiluminogens – 10-Methyl-9-thiophenoxycarbonylacridinium Cations. *Int. J. Mol. Sci.* **2020**, *21*, 4417. https://doi.org/10.3390/ijms21124417.

Figure S2. The diagram of relative free energy in aqueous phase of the first steps of reaction leading to the light emission (step I, Scheme 1) and competitive reactions (step IV – formation of 'pseudobase' and step V – formation of 10-methyl-9-carboxyacridinium acid (hydrolysis of the compound)) of the selected acridinium R-esters (Table 1).

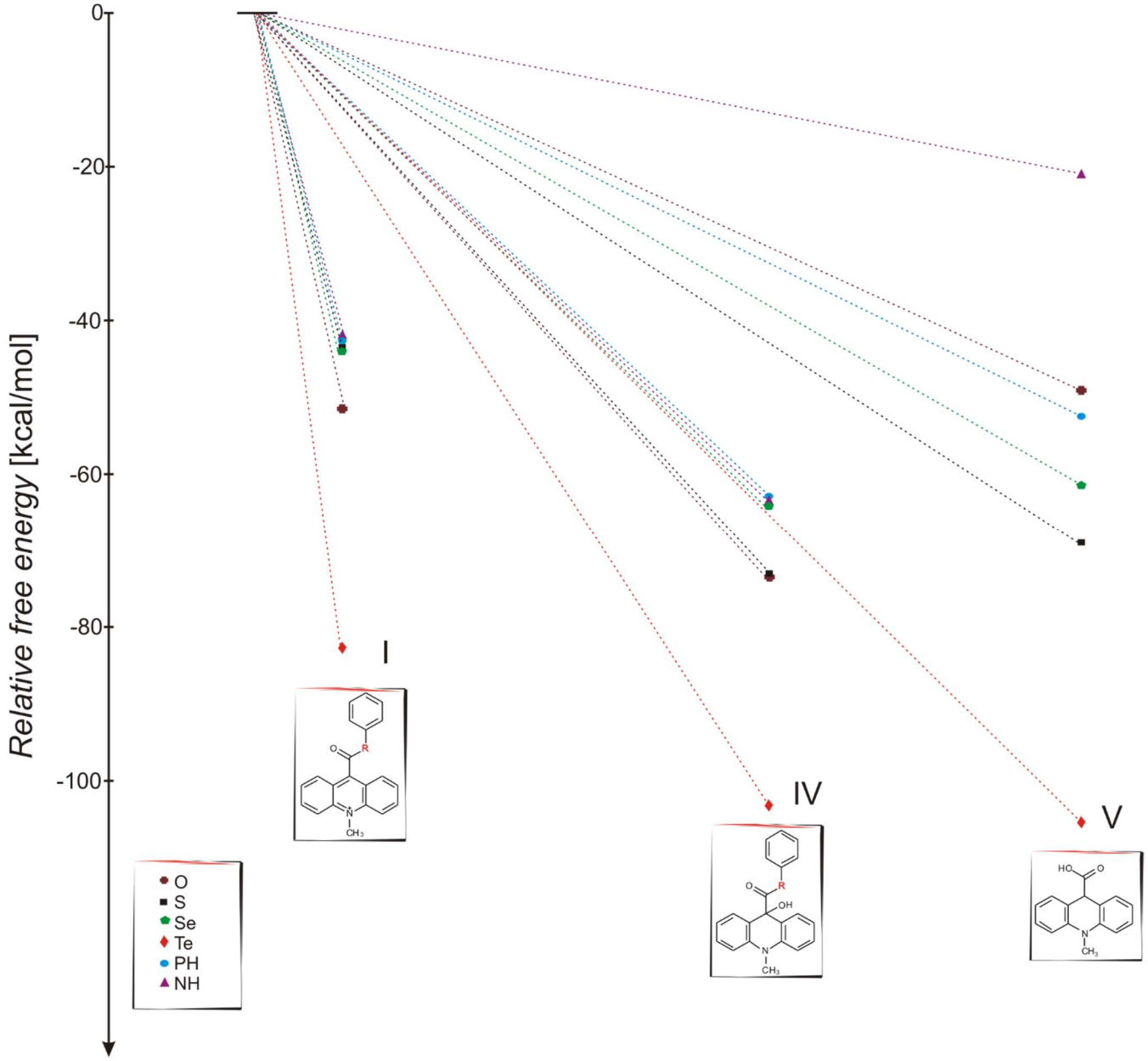
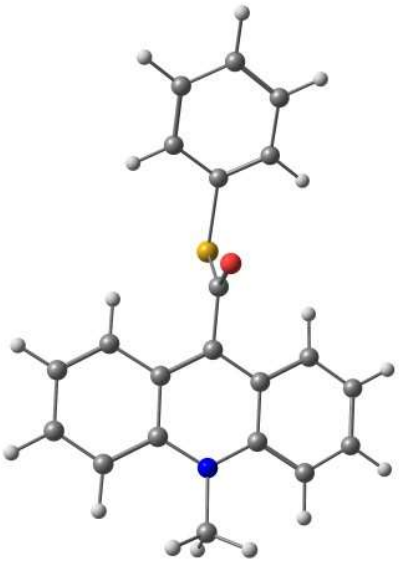
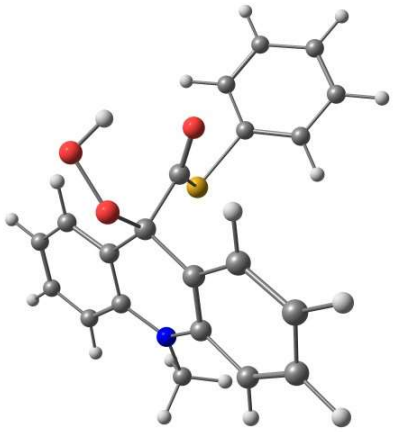


Table S2. Cartesian coordinates and structures of the lowest energy structures of investigated molecules. List of abbreviations: * – excited product, S_1 – first singlet state.

R = Se			
Structure no. 1 *E* = –3339.05392109 Ha			
Atom	X	Y	Z
C	3.026493000	1.205623000	0.132682000
C	3.718741000	2.438874000	0.067188000
C	3.014903000	3.620651000	-0.037465000
C	1.600712000	3.642912000	-0.091613000
C	0.904764000	2.464152000	-0.037858000
C	1.590978000	1.219195000	0.084490000
H	4.799042000	2.472951000	0.058936000
H	3.565464000	4.553752000	-0.100840000
H	1.077864000	4.586895000	-0.196166000
H	-0.173409000	2.442833000	-0.144760000
C	0.896503000	-0.000046000	0.146445000
C	1.591220000	-1.219134000	0.084562000
C	3.026745000	-1.205252000	0.132718000
N	3.688225000	0.000254000	0.251494000
C	-0.595391000	-0.000038000	0.426849000
C	5.142636000	0.000343000	0.513242000
C	0.905271000	-2.464256000	-0.037690000
C	1.601474000	-3.642866000	-0.091471000
C	3.015659000	-3.620288000	-0.037405000
C	3.719251000	-2.438360000	0.067231000
H	-0.172903000	-2.443186000	-0.144586000
H	1.078830000	-4.586966000	-0.195994000
H	3.566430000	-4.553262000	-0.100846000
H	4.799559000	-2.472192000	0.058952000
H	5.400583000	0.876162000	1.102711000
H	5.400579000	-0.875196000	1.103142000
H	5.709299000	0.000143000	-0.421747000
Se	-1.714309000	-0.000537000	-1.132899000
O	-0.969538000	0.000408000	1.575058000
C	-3.423868000	-0.000150000	-0.255519000
C	-4.043887000	1.216285000	0.039046000
C	-5.298761000	1.211153000	0.647571000
C	-5.923269000	0.000248000	0.952905000
C	-5.298646000	-1.210868000	0.648609000
C	-4.043804000	-1.216391000	0.040057000
H	-3.558192000	2.153953000	-0.208634000
H	-5.787755000	2.151717000	0.880376000
H	-6.900928000	0.000411000	1.424378000
H	-5.787548000	-2.151287000	0.882193000
H	-3.558014000	-2.154209000	-0.206901000



R = Se			
Structure no. 2 *E* = –3490.21432860 Ha			
Atom	X	Y	Z
C	1.454506000	-2.450311000	0.884827000
C	1.642049000	-1.134024000	0.437317000
C	2.477137000	-0.898320000	-0.678658000
C	3.153006000	-1.991721000	-1.258926000
C	2.963359000	-3.283097000	-0.783534000
C	2.102922000	-3.524236000	0.287678000
C	0.951421000	0.003732000	1.163136000
C	1.382167000	1.366696000	0.650542000
C	2.206698000	1.507822000	-0.485372000
N	2.634749000	0.389700000	-1.202428000
C	2.602405000	2.807630000	-0.865058000
C	2.155662000	3.923783000	-0.168424000
C	1.312849000	3.783729000	0.935243000
C	0.941261000	2.506386000	1.335504000
C	-0.592927000	-0.071091000	1.014365000
O	-1.371123000	0.283209000	1.866980000
O	1.281443000	0.070220000	2.572143000
O	0.594091000	-0.969624000	3.322573000
C	3.230423000	0.565038000	-2.520884000
Se	-1.111786000	-0.723849000	-0.746682000
C	-2.970695000	-0.234969000	-0.631562000
C	-3.389725000	1.023464000	-1.071449000
C	-4.741076000	1.364774000	-1.011220000
C	-5.671844000	0.451179000	-0.513099000
C	-5.251199000	-0.805174000	-0.073750000
C	-3.900568000	-1.150380000	-0.132728000
H	3.284802000	2.948298000	-1.693362000
H	2.481267000	4.909538000	-0.487907000
H	0.960658000	4.653252000	1.480040000
H	0.299948000	2.368078000	2.198026000
H	0.803203000	-2.612586000	1.734129000
H	1.944216000	-4.532171000	0.656451000
H	3.499514000	-4.102811000	-1.253018000
H	3.851688000	-1.831532000	-2.069949000
H	2.793191000	1.439613000	-3.003660000
H	4.320866000	0.690224000	-2.485186000
H	2.996861000	-0.299176000	-3.143258000
H	-3.567360000	-2.125283000	0.207623000
H	-5.972864000	-1.517044000	0.316069000
H	-6.723647000	0.717961000	-0.467766000
H	-5.065321000	2.343733000	-1.351895000
H	-2.661385000	1.730438000	-1.455323000
H	-0.270411000	-0.533479000	3.445918000



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C	-1.200325000	-2.179999000	0.000000000
C	0.000000000	-2.900719000	0.000000000
C	1.200325000	-2.179999000	0.000000000
C	1.198754000	-0.787256000	0.000000000
H	-2.140954000	-0.245081000	0.000000000
H	2.140954000	-0.245081000	0.000000000
Se	0.000000000	1.855686000	0.000000000
H	-2.151472000	-2.713114000	0.000000000
H	0.000000000	-3.988703000	0.000000000
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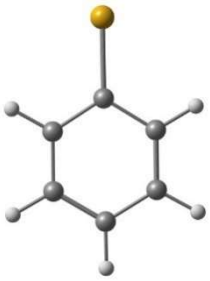
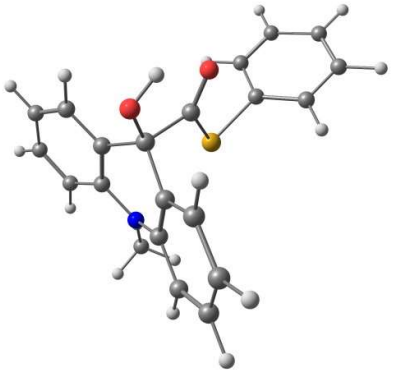


R = Se			
Structure no. 6 *E* = –3415.08976629 Ha			
Atom	X	Y	Z
C	3.631695000	-1.211021000	-0.336270000
C	2.942199000	-0.000020000	-0.436718000
C	3.631719000	1.210988000	-0.336522000
C	5.012411000	1.209013000	-0.135834000
C	5.702874000	-0.000002000	-0.035776000
C	5.012370000	-1.209030000	-0.135591000
Se	1.044003000	0.000124000	-0.759201000
C	0.490016000	0.000156000	1.098656000
O	1.269093000	0.000220000	2.024594000
C	-1.057390000	-0.000025000	1.374159000
C	-1.675618000	-1.247725000	0.754770000
C	-2.123352000	-1.210268000	-0.581335000
N	-2.051452000	-0.000051000	-1.295081000
C	-2.123503000	1.210118000	-0.581290000
C	-1.675752000	1.247604000	0.754811000
C	-1.765980000	-2.431654000	1.484460000
C	-2.269827000	-3.594967000	0.904653000
C	-2.696353000	-3.563245000	-0.422586000
C	-2.635547000	-2.382333000	-1.160324000
C	-2.635766000	2.382166000	-1.160275000
C	-2.696600000	3.563090000	-0.422561000
C	-2.270037000	3.594846000	0.904665000
C	-1.766138000	2.431556000	1.484466000
C	-2.196153000	-0.000047000	-2.739897000
H	-3.014150000	-2.370708000	-2.175542000
H	-3.098563000	-4.457838000	-0.889251000
H	-2.328015000	-4.512441000	1.481445000
H	-1.438581000	-2.420351000	2.518059000
H	-1.438681000	2.420291000	2.518049000
H	-2.328194000	4.512328000	1.481447000
H	-3.098866000	4.457653000	-0.889234000
H	-3.014353000	2.370492000	-2.175497000
H	-1.698938000	-0.882299000	-3.147515000
H	-3.243525000	0.000042000	-3.075167000
H	-1.698775000	0.882112000	-3.147537000
H	3.090590000	2.148337000	-0.414389000
H	5.546609000	2.151244000	-0.056695000
H	6.777793000	-0.000028000	0.119303000
H	5.546587000	-2.151238000	-0.056286000
H	3.090504000	-2.148356000	-0.413936000
O	-1.206438000	0.000011000	2.776686000
H	-0.300204000	-0.000153000	3.136915000



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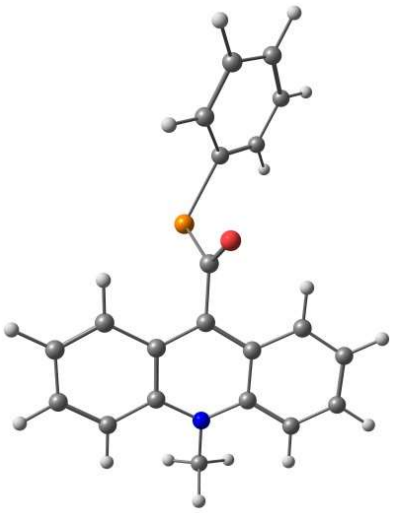
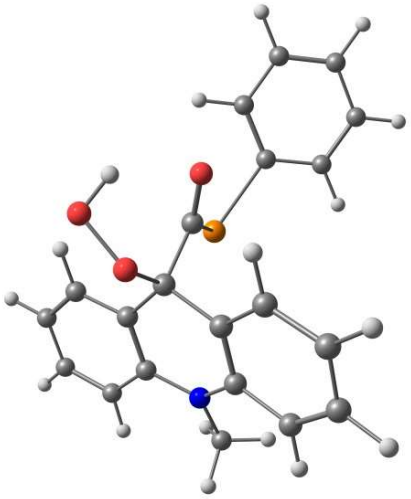
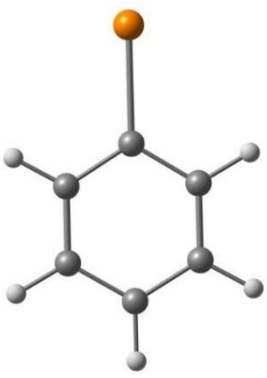
Atom	X	Y	Z
C	-4.062906000	-0.842494000	0.983458000
C	-3.383205000	0.115720000	0.220410000
C	-3.928313000	0.588652000	-0.979511000
C	-5.155338000	0.088819000	-1.418856000
C	-5.839760000	-0.861856000	-0.659461000
C	-5.296094000	-1.323654000	0.541018000
Te	-1.516203000	0.870465000	0.919442000
C	-0.405409000	0.003896000	-0.768783000
O	-0.939575000	-0.430581000	-1.758631000
C	1.081673000	-0.104461000	-0.531125000
C	1.652757000	-1.384340000	-0.357479000
C	3.035789000	-1.482067000	0.021711000
N	3.767743000	-0.330291000	0.233832000
C	3.270979000	0.914748000	-0.090432000
C	1.890731000	1.047924000	-0.471736000
C	3.618642000	-2.764407000	0.165750000
C	2.857724000	-3.897157000	-0.033505000
C	1.488223000	-3.813951000	-0.376499000
C	0.900924000	-2.585291000	-0.536672000
C	4.089219000	2.069944000	-0.067151000
C	3.561879000	3.300446000	-0.400271000
C	2.206419000	3.446444000	-0.774701000
C	1.392619000	2.342952000	-0.813689000
C	5.119354000	-0.435341000	0.821490000
H	4.669283000	-2.875753000	0.394055000
H	3.327519000	-4.870497000	0.066615000
H	0.911389000	-4.719898000	-0.526178000
H	-0.138213000	-2.510542000	-0.830181000
H	0.361334000	2.437815000	-1.131035000
H	1.820792000	4.422423000	-1.047642000
H	4.211774000	4.169770000	-0.392550000
H	5.142060000	2.001860000	0.168156000
H	5.150540000	-1.285411000	1.498130000
H	5.879400000	-0.550307000	0.043672000
H	5.324755000	0.455048000	1.410117000
H	-3.407854000	1.335974000	-1.568040000
H	-5.578132000	0.450134000	-2.351339000
H	-6.797868000	-1.240968000	-1.001575000
H	-5.827604000	-2.062397000	1.133202000
H	-3.639672000	-1.211906000	1.912026000



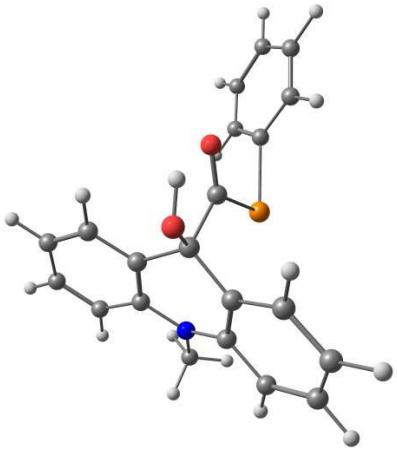
R = Te			
Structure no. 2 *E* = –1098.83706374 Ha			
Atom	X	Y	Z
C	-3.876335000	-0.736580000	0.549231000
C	-3.112692000	-0.241706000	-0.514872000
C	-3.675268000	0.687390000	-1.399091000
C	-4.994473000	1.110699000	-1.223496000
C	-5.751976000	0.621452000	-0.158117000
C	-5.189864000	-0.297929000	0.728989000
Te	-1.103457000	-0.914530000	-0.818285000
C	-0.412169000	-0.049869000	1.091938000
O	-1.179005000	0.290034000	1.957681000
C	1.135954000	0.124449000	1.216156000
C	1.904986000	-0.985753000	0.528420000
C	2.711012000	-0.728919000	-0.606344000
N	2.757941000	0.545094000	-1.183059000
C	2.277417000	1.656537000	-0.487484000
C	1.472955000	1.497214000	0.660997000
C	3.470197000	-1.786164000	-1.149999000
C	3.403862000	-3.065246000	-0.611102000
C	2.588947000	-3.328418000	0.490269000
C	1.855987000	-2.288357000	1.050340000
C	2.587603000	2.966076000	-0.910671000
C	2.084188000	4.072745000	-0.237272000
C	1.265197000	3.913342000	0.882152000
C	0.974567000	2.627968000	1.322425000
O	1.468211000	0.260069000	2.619940000
O	0.862909000	-0.796728000	3.415414000
C	3.327506000	0.717903000	-2.513066000
H	3.249166000	3.123442000	-1.753043000
H	2.344563000	5.067156000	-0.588622000
H	0.867710000	4.775433000	1.407494000
H	0.350921000	2.477030000	2.195708000
H	1.241333000	-2.465678000	1.923589000
H	2.531230000	-4.326159000	0.912818000
H	4.002568000	-3.856546000	-1.053284000
H	4.140776000	-1.603518000	-1.979988000
H	2.824243000	1.542867000	-3.018846000
H	4.406767000	0.921443000	-2.494683000
H	3.150327000	-0.181360000	-3.103927000
H	-3.450007000	-1.458783000	1.236903000
H	-5.774891000	-0.681461000	1.560305000
H	-6.776308000	0.955540000	-0.019608000
H	-5.424927000	1.830065000	-1.914687000
H	-3.086280000	1.086424000	-2.219254000
H	-0.025538000	-0.413998000	3.540663000



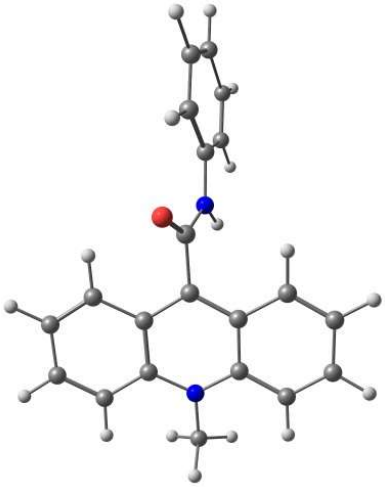
R = Te			
Structure no. 4 *E* = –239.746242242 Ha			
Atom	X	Y	Z
C	1.199037000	-1.287224000	0.000000000
C	0.000000000	-0.540690000	0.000000000
C	-1.199037000	-1.287224000	0.000000000
C	-1.201319000	-2.682991000	0.000000000
C	0.000000000	-3.399270000	0.000000000
C	1.201319000	-2.682991000	0.000000000
Te	0.000000000	1.609792000	0.000000000
H	-2.145083000	-0.752178000	0.000000000
H	2.145083000	-0.752178000	0.000000000
H	-2.151326000	-3.217499000	0.000000000
H	0.000000000	-4.487469000	0.000000000
H	2.151326000	-3.217498000	0.000000000



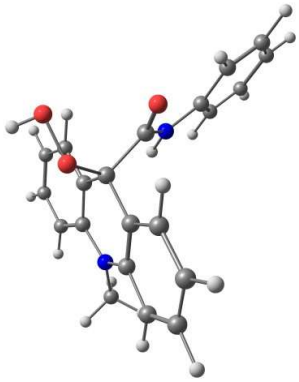
R = Te			
Structure no. 6 *E* = –1023.71267584 Ha			
Atom	X	Y	Z
C	3.734260000	0.780390000	-1.135010000
C	3.090615000	-0.212319000	-0.386001000
C	3.794953000	-0.895515000	0.612722000
C	5.132087000	-0.580615000	0.862362000
C	5.775545000	0.402730000	0.109074000
C	5.076353000	1.080209000	-0.890969000
Te	1.049899000	-0.699944000	-0.801707000
C	0.360494000	-0.029172000	1.168927000
O	1.134585000	0.215114000	2.062978000
C	-1.190297000	0.124116000	1.416403000
C	-1.624061000	1.450986000	0.801574000
C	-2.247030000	1.494687000	-0.463451000
N	-2.503722000	0.304777000	-1.160179000
C	-2.576138000	-0.906673000	-0.456280000
C	-1.964793000	-1.029399000	0.811279000
C	-2.616218000	2.746168000	-0.992367000
C	-2.351454000	3.919259000	-0.291337000
C	-1.733487000	3.875684000	0.958931000
C	-1.382987000	2.639492000	1.494440000
C	-3.268210000	-2.016312000	-0.980472000
C	-3.333145000	-3.212557000	-0.272394000
C	-2.732330000	-3.331266000	0.981844000
C	-2.061785000	-2.234110000	1.513577000
O	-1.353127000	0.133908000	2.823359000
C	-2.905139000	0.358297000	-2.556777000
H	-3.786075000	-1.938523000	-1.928481000
H	-3.875210000	-4.050699000	-0.701170000
H	-2.790778000	-4.261266000	1.538151000
H	-1.606397000	-2.285145000	2.496374000
H	-0.920504000	2.579247000	2.473591000
H	-1.532611000	4.788718000	1.510148000
H	-2.647736000	4.871075000	-0.723057000
H	-3.138202000	2.806919000	-1.939492000
H	-2.624818000	-0.573352000	-3.050803000
H	-3.984952000	0.515745000	-2.692184000
H	-2.368950000	1.168000000	-3.054599000
H	3.191504000	1.323882000	-1.902180000
H	5.570380000	1.849934000	-1.477375000
H	6.817955000	0.640508000	0.301083000
H	5.671403000	-1.109920000	1.642942000
H	3.304434000	-1.667074000	1.196178000
H	-0.463190000	0.268930000	3.193744000



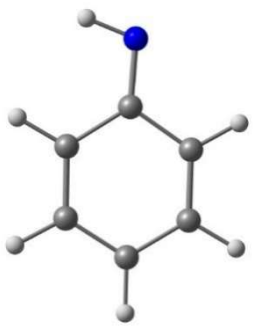
R = NH			
Structure no. 1 *E* = –995.042190249 Ha			
Atom	X	Y	Z
C	3.983850000	-0.383659000	-0.841398000
C	3.251501000	0.012528000	0.285383000
C	3.909955000	0.351376000	1.475278000
C	5.298594000	0.294023000	1.542142000
C	6.038038000	-0.101793000	0.425929000
C	5.375407000	-0.437120000	-0.754691000
N	1.829882000	0.100708000	0.293932000
C	0.949836000	-0.261921000	-0.676232000
O	1.217949000	-0.708892000	-1.783532000
C	-0.516275000	-0.089663000	-0.304170000
C	-1.094867000	1.193144000	-0.253189000
C	-2.490151000	1.322634000	0.070234000
N	-3.224646000	0.193429000	0.364323000
C	-2.707729000	-1.075443000	0.192656000
C	-1.319428000	-1.235564000	-0.143613000
C	-0.340062000	2.373876000	-0.533918000
C	-0.929021000	3.611012000	-0.510808000
C	-2.307182000	3.722006000	-0.211765000
C	-3.074739000	2.612841000	0.072648000
C	-3.514829000	-2.229793000	0.338132000
C	-2.962890000	-3.483462000	0.182274000
C	-1.592125000	-3.655052000	-0.121893000
C	-0.791374000	-2.555245000	-0.285558000
C	-4.600119000	0.343213000	0.884085000
H	-4.131699000	2.745515000	0.254542000
H	-2.779528000	4.699015000	-0.220306000
H	-0.350592000	4.499297000	-0.738470000
H	0.707358000	2.273125000	-0.792351000
H	0.248191000	-2.669093000	-0.566045000
H	-1.185013000	-4.652628000	-0.242596000
H	-3.602039000	-4.354697000	0.283354000
H	-4.574414000	-2.148835000	0.534121000
H	-4.672581000	1.268079000	1.449436000
H	-5.329363000	0.346352000	0.069567000
H	-4.814909000	-0.472256000	1.569622000
H	3.336806000	0.657124000	2.347928000
H	5.800607000	0.558099000	2.467309000
H	7.120844000	-0.147022000	0.477069000
H	5.943453000	-0.743985000	-1.627215000
H	3.474007000	-0.642440000	-1.758300000
H	1.430297000	0.428906000	1.163651000



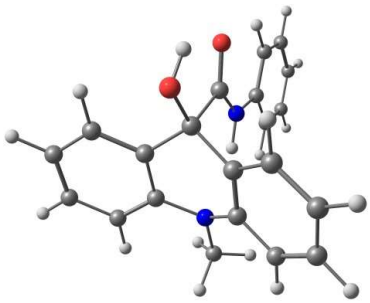
R = NH			
Structure no. 2			
E = –1146.19582424 Ha			
Atom	X	Y	Z
C	0.427008000	-2.323719000	1.107160000
C	1.018929000	-1.198068000	0.507799000
C	1.995006000	-1.396079000	-0.499763000
C	2.406786000	-2.715336000	-0.790318000
C	1.824833000	-3.806328000	-0.157111000
C	0.812265000	-3.620905000	0.783887000
C	0.651624000	0.191284000	0.996718000
C	1.368847000	1.289496000	0.229259000
C	2.299359000	1.002319000	-0.790972000
N	2.526473000	-0.316604000	-1.208413000
C	3.001108000	2.073911000	-1.380530000
C	2.760506000	3.385982000	-0.989868000
C	1.825766000	3.670548000	0.005446000
C	1.149172000	2.619504000	0.612955000
C	-0.888107000	0.491490000	0.994458000
O	-1.379907000	1.281707000	1.782604000
O	1.156575000	0.424200000	2.338566000
O	0.470163000	-0.427343000	3.297450000
C	3.271000000	-0.560587000	-2.438168000
N	-1.573292000	-0.138185000	-0.013289000
C	-2.929764000	-0.008807000	-0.379137000
C	-3.371363000	-0.765464000	-1.476517000
C	-4.694746000	-0.688544000	-1.899595000
C	-5.598303000	0.143046000	-1.235746000
C	-5.157144000	0.892574000	-0.144973000
C	-3.834502000	0.827159000	0.293242000
H	3.762247000	1.884825000	-2.126344000
H	3.320453000	4.187548000	-1.462938000
H	1.638098000	4.693279000	0.315114000
H	0.432866000	2.806571000	1.404294000
H	-0.351956000	-2.161936000	1.842539000
H	0.335809000	-4.469162000	1.264173000
H	2.167300000	-4.806398000	-0.406590000
H	3.205300000	-2.892243000	-1.499080000
H	3.103043000	0.261137000	-3.134703000
H	4.351079000	-0.664837000	-2.271033000
H	2.901481000	-1.468350000	-2.915727000
H	-3.494001000	1.404887000	1.140315000
H	-5.850587000	1.542277000	0.381369000
H	-6.631173000	0.204326000	-1.564204000
H	-5.017968000	-1.280823000	-2.750726000
H	-2.671705000	-1.414441000	-1.998616000
H	1.161179000	-1.092883000	3.454638000
H	-1.038056000	-0.799626000	-0.558892000



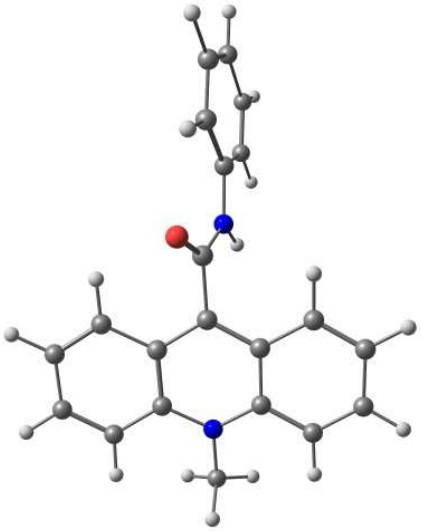
R = NH			
Structure no. 4			
E = –475.635065838 Ha			
Atom	X	Y	Z
C	-1.205093000	0.259174000	0.000000000
C	0.000000000	1.067518000	0.000000000
C	1.217134000	0.278160000	0.000000000
C	1.215187000	-1.105164000	0.000000000
C	0.020466000	-1.852412000	0.000000000
C	-1.182463000	-1.128312000	0.000000000
N	0.064416000	2.395719000	0.000000000
H	2.156402000	0.829887000	0.000000000
H	-2.165453000	0.780130000	0.000000000
H	2.172952000	-1.631243000	0.000000000
H	0.029689000	-2.940028000	0.000000000
H	-2.132514000	-1.668681000	0.000000000
H	-0.903369000	2.746120000	0.000000000



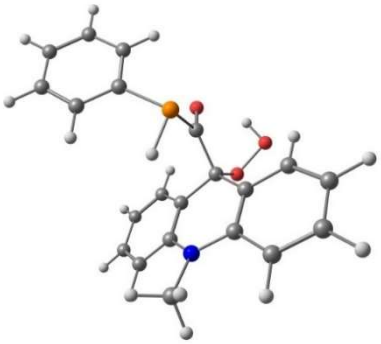
R = NH			
Structure no. 6 *E* = –1071.08223898 Ha			
Atom	X	Y	Z
C	1.706569000	2.418117000	-1.297183000
C	1.437738000	1.244530000	-0.595370000
C	1.612636000	1.210492000	0.802018000
C	2.045982000	2.367449000	1.466387000
C	2.288376000	3.539362000	0.749905000
C	2.123730000	3.571111000	-0.633445000
C	0.938389000	-0.000139000	-1.326449000
C	1.438131000	-1.244361000	-0.595128000
C	1.613126000	-1.209983000	0.802246000
N	1.331895000	0.000263000	1.492743000
C	2.047033000	-2.366627000	1.466790000
C	2.289719000	-3.538629000	0.750548000
C	2.124849000	-3.570748000	-0.632766000
C	1.707229000	-2.418034000	-1.296694000
C	-0.636648000	-0.000358000	-1.384714000
O	-1.176750000	-0.000385000	-2.490087000
O	1.362220000	-0.000223000	-2.667482000
C	1.378376000	0.000469000	2.947929000
N	-1.286279000	-0.000587000	-0.193345000
C	-2.676837000	-0.000429000	0.059540000
C	-3.648309000	-0.000596000	-0.952397000
C	-4.998427000	-0.000462000	-0.601654000
C	-5.399916000	-0.000169000	0.734208000
C	-4.428895000	-0.000013000	1.736985000
C	-3.077677000	-0.000149000	1.404631000
H	2.221831000	-2.356655000	2.535716000
H	2.625647000	-4.423582000	1.283048000
H	2.322338000	-4.480634000	-1.190481000
H	1.590932000	-2.404007000	-2.374388000
H	1.590392000	2.403813000	-2.374883000
H	2.321048000	4.480939000	-1.191318000
H	2.623881000	4.424571000	1.282250000
H	2.220543000	2.357815000	2.535354000
H	0.857729000	-0.882118000	3.323403000
H	2.401915000	0.000837000	3.350376000
H	0.857206000	0.882863000	3.323163000
H	-2.325129000	-0.000022000	2.189527000
H	-4.721190000	0.000215000	2.782942000
H	-6.454440000	-0.000084000	0.991650000
H	-5.744070000	-0.000594000	-1.391443000
H	-3.340731000	-0.000799000	-1.988135000
H	0.529379000	-0.000092000	-3.184231000
H	-0.691400000	-0.000335000	0.629902000



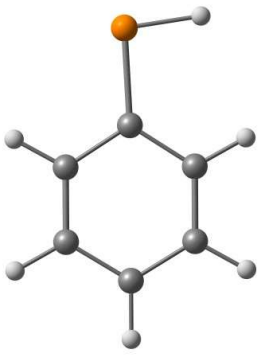
R = PH			
Structure no. 1 *E* = –1281.60578101 Ha			
Atom	X	Y	Z
C	4.127088000	1.001038000	-0.611699000
C	3.299225000	0.682260000	0.477088000
C	3.751661000	-0.221049000	1.452428000
C	5.015421000	-0.797885000	1.335933000
C	5.829196000	-0.489625000	0.243665000
C	5.382250000	0.405494000	-0.729700000
P	1.679913000	1.520125000	0.625132000
C	0.718028000	0.675839000	-0.761818000
O	1.182791000	0.547574000	-1.876249000
C	-0.690223000	0.208588000	-0.451901000
C	-1.725807000	1.136345000	-0.230076000
C	-3.021675000	0.658331000	0.169742000
N	-3.215110000	-0.693823000	0.363842000
C	-2.253570000	-1.622916000	0.018933000
C	-0.949014000	-1.175886000	-0.385033000
C	-1.536478000	2.540157000	-0.418002000
C	-2.566361000	3.424232000	-0.224264000
C	-3.839016000	2.938910000	0.154040000
C	-4.070042000	1.592884000	0.346962000
C	-2.522182000	-3.012522000	0.047991000
C	-1.533534000	-3.915547000	-0.281828000
C	-0.236658000	-3.489205000	-0.649805000
C	0.046708000	-2.149033000	-0.704051000
C	-4.484148000	-1.162630000	0.958174000
H	-5.070382000	1.267652000	0.594825000
H	-4.661240000	3.635759000	0.280963000
H	-2.414128000	4.486545000	-0.377843000
H	-0.566370000	2.899948000	-0.739379000
H	1.026621000	-1.810054000	-1.015818000
H	0.522510000	-4.220533000	-0.903316000
H	-1.764890000	-4.975757000	-0.267260000
H	-3.507463000	-3.384746000	0.290079000
H	-4.867177000	-0.402901000	1.633863000
H	-5.224626000	-1.379407000	0.183518000
H	-4.294744000	-2.055084000	1.548849000
H	3.124169000	-0.470921000	2.303205000
H	5.362361000	-1.490468000	2.096515000
H	6.812050000	-0.941713000	0.155110000
H	6.015034000	0.650445000	-1.576827000
H	3.793212000	1.705943000	-1.366027000
H	1.114586000	0.792905000	1.704994000



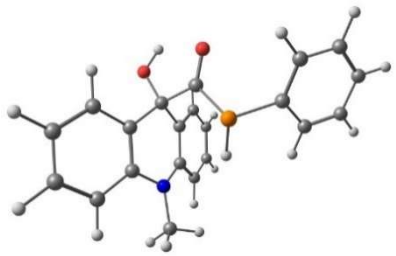
R = PH			
Structure no. 2			
E = –1281.60578101 Ha			
Atom	X	Y	Z
C	-3.756188000	-1.510813000	-0.168238000
C	-2.815159000	-0.741113000	-0.869776000
C	-3.244520000	0.416295000	-1.536550000
C	-4.586368000	0.795544000	-1.501950000
C	-5.513441000	0.031452000	-0.791510000
C	-5.093762000	-1.118682000	-0.121566000
P	-1.072843000	-1.323975000	-0.967708000
C	-0.510968000	-1.020398000	0.809739000
O	-1.203338000	-1.394561000	1.739729000
C	0.879069000	-0.360488000	1.045012000
C	1.933862000	-0.880111000	0.083812000
C	2.555443000	-0.028012000	-0.858069000
N	2.138826000	1.302254000	-1.011738000
C	1.337000000	1.913874000	-0.044394000
C	0.684746000	1.143593000	0.941629000
C	3.598231000	-0.543851000	-1.653214000
C	3.978392000	-1.877608000	-1.557274000
C	3.337154000	-2.731765000	-0.662149000
C	2.328742000	-2.224041000	0.150350000
C	1.154518000	3.312352000	-0.027919000
C	0.320557000	3.913237000	0.908230000
C	-0.349153000	3.146642000	1.862330000
C	-0.152415000	1.770856000	1.873145000
O	1.259335000	-0.519483000	2.435940000
O	1.188260000	-1.909721000	2.858068000
C	2.579716000	2.067042000	-2.170309000
H	1.688521000	3.940385000	-0.729372000
H	0.204469000	4.993101000	0.893310000
H	-1.003091000	3.612931000	2.591478000
H	-0.643078000	1.153252000	2.616604000
H	1.847113000	-2.863383000	0.878843000
H	3.623446000	-3.775596000	-0.587755000
H	4.785850000	-2.243547000	-2.184784000
H	4.136234000	0.103786000	-2.333561000
H	1.817388000	2.801396000	-2.432667000
H	3.530021000	2.591803000	-2.003041000
H	2.694927000	1.398832000	-3.024305000
H	-3.441068000	-2.410017000	0.350981000
H	-5.809885000	-1.717781000	0.433333000
H	-6.557154000	0.330118000	-0.761569000
H	-4.904749000	1.693881000	-2.023087000
H	-2.529459000	1.028318000	-2.079047000
H	0.225408000	-1.973689000	3.010822000
H	-0.490810000	-0.173836000	-1.556258000



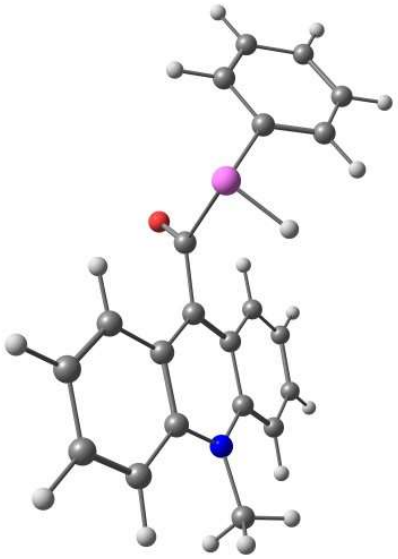
R = PH			
Structure no. 4			
E = –573.614541130 Ha			
Atom	X	Y	Z
C	-1.201510000	-0.185798000	0.000000000
C	0.000000000	0.582890000	0.000000000
C	1.199484000	-0.191065000	0.000000000
C	1.197356000	-1.579832000	0.000000000
C	-0.003832000	-2.305165000	0.000000000
C	-1.200914000	-1.576831000	0.000000000
P	0.093148000	2.390918000	0.000000000
H	2.153317000	0.335049000	0.000000000
H	-2.153794000	0.340997000	0.000000000
H	2.149223000	-2.112640000	0.000000000
H	-0.005571000	-3.392764000	0.000000000
H	-2.154572000	-2.106835000	0.000000000
H	-1.329325000	2.607235000	0.000000000



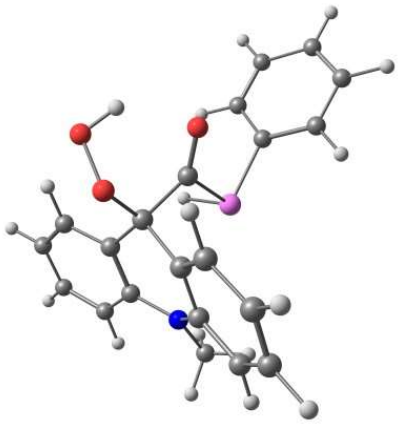
R = PH			
Structure no. 6			
E = −1357.64293927 Ha			
Atom	X	Y	Z
C	0.155033000	2.045870000	-1.888151000
C	0.794914000	1.214380000	-0.967185000
C	1.293277000	1.758537000	0.235276000
C	1.137870000	3.138020000	0.468336000
C	0.480441000	3.944876000	-0.456672000
C	-0.017062000	3.405386000	-1.642338000
C	0.932670000	-0.273408000	-1.277344000
C	2.050131000	-0.894022000	-0.452478000
C	2.503713000	-0.284280000	0.736550000
N	1.936416000	0.927173000	1.167816000
C	3.537137000	-0.906598000	1.462062000
C	4.084186000	-2.111090000	1.028586000
C	3.634750000	-2.713456000	-0.146145000
C	2.628234000	-2.091855000	-0.879337000
C	-0.434590000	-0.983683000	-0.959600000
O	-1.081334000	-1.427010000	-1.893561000
O	1.166885000	-0.475115000	-2.656564000
C	2.241933000	1.432705000	2.496271000
P	-1.003333000	-1.301414000	0.801115000
C	-2.775538000	-0.822388000	0.674925000
C	-3.667755000	-1.675188000	0.006787000
C	-5.024925000	-1.361821000	-0.061264000
C	-5.511857000	-0.207856000	0.554653000
C	-4.633060000	0.639309000	1.231261000
C	-3.272001000	0.338580000	1.286306000
H	3.939530000	-0.437902000	2.351462000
H	4.880356000	-2.568261000	1.608946000
H	4.066320000	-3.647922000	-0.489715000
H	2.279272000	-2.519280000	-1.812954000
H	-0.196080000	1.605350000	-2.814812000
H	-0.523836000	4.033685000	-2.367534000
H	0.375309000	5.006215000	-0.250926000
H	1.556316000	3.593102000	1.357528000
H	2.301325000	0.597154000	3.195599000
H	3.185586000	1.995371000	2.541639000
H	1.433031000	2.084837000	2.829540000
H	-2.594417000	1.015088000	1.799333000
H	-5.004027000	1.541490000	1.709118000
H	-6.570565000	0.029716000	0.508402000
H	-5.703486000	-2.024908000	-0.589927000
H	-3.299546000	-2.578439000	-0.468962000
H	0.359096000	-0.911597000	-2.990473000
H	-0.498530000	-0.117809000	1.390318000



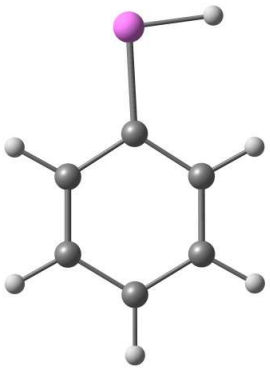
R = AsH			
Structure no. 1 *E* = –3174.02151596 Ha			
Atom	X	Y	Z
C	3.473450000	0.680713000	-1.212221000
C	3.190453000	-0.434580000	-0.412517000
C	4.116812000	-0.843946000	0.555945000
C	5.308377000	-0.140149000	0.728295000
C	5.587800000	0.966717000	-0.074388000
C	4.671591000	1.374428000	-1.046521000
As	1.563073000	-1.464537000	-0.587153000
C	0.568711000	-0.479291000	0.866390000
O	1.079418000	-0.239365000	1.935722000
C	-0.847856000	-0.067205000	0.540265000
C	-1.154616000	1.302470000	0.410719000
C	-2.469886000	1.683597000	-0.025266000
N	-3.392975000	0.706221000	-0.340895000
C	-3.149723000	-0.630302000	-0.097430000
C	-1.842774000	-1.042951000	0.333776000
C	-2.789081000	3.060058000	-0.111703000
C	-1.836570000	4.011319000	0.187861000
C	-0.527243000	3.648542000	0.579023000
C	-0.195470000	2.323105000	0.691187000
C	-4.158981000	-1.611048000	-0.252664000
C	-3.877160000	-2.939735000	-0.013231000
C	-2.590049000	-3.361339000	0.391354000
C	-1.598538000	-2.431051000	0.568525000
C	-4.674120000	1.103472000	-0.960611000
H	-5.168681000	-1.334778000	-0.521345000
H	-4.669438000	-3.672781000	-0.125710000
H	-2.397584000	-4.411475000	0.579730000
H	-0.617845000	-2.742364000	0.908232000
H	0.796429000	2.032433000	1.012899000
H	0.203810000	4.417304000	0.802687000
H	-2.106246000	5.060848000	0.127940000
H	-3.784662000	3.386068000	-0.377239000
H	-5.018733000	0.307759000	-1.615231000
H	-5.430604000	1.313750000	-0.199752000
H	-4.515796000	1.983686000	-1.577967000
H	2.768336000	1.004646000	-1.972096000
H	4.889273000	2.231994000	-1.675792000
H	6.520164000	1.507822000	0.052941000
H	6.019718000	-0.462070000	1.482179000
H	3.910244000	-1.710730000	1.176920000
H	0.904941000	-0.647963000	-1.682569000



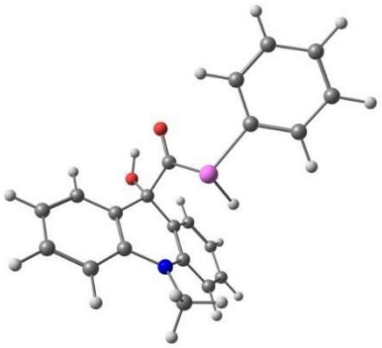
R = AsH			
Structure no. 2			
E = –3325.18494918 Ha			
Atom	X	Y	Z
C	1.552862000	2.429297000	1.502510000
C	1.609710000	1.271973000	0.718769000
C	2.115524000	1.340329000	-0.596989000
C	2.568414000	2.578767000	-1.085354000
C	2.508170000	3.718020000	-0.288530000
C	2.002334000	3.651316000	1.010214000
C	1.041861000	-0.044292000	1.241155000
C	1.685322000	-1.232701000	0.537911000
C	2.199609000	-1.071736000	-0.766785000
N	2.152531000	0.187645000	-1.387509000
C	2.761321000	-2.178237000	-1.426437000
C	2.807420000	-3.422384000	-0.804497000
C	2.311838000	-3.581863000	0.488685000
C	1.757849000	-2.487631000	1.150441000
C	-0.491086000	0.063671000	0.962835000
O	-1.276441000	0.361970000	1.835091000
O	1.292914000	-0.015277000	2.653447000
O	0.456811000	-0.975041000	3.357348000
C	2.287231000	0.293333000	-2.831030000
As	-1.062033000	-0.108443000	-0.974176000
C	-2.969375000	-0.090217000	-0.603794000
C	-3.638413000	1.139268000	-0.654568000
C	-5.005240000	1.221991000	-0.388275000
C	-5.724799000	0.068988000	-0.073506000
C	-5.070378000	-1.162711000	-0.020702000
C	-3.701450000	-1.238190000	-0.277028000
H	2.993446000	2.646801000	-2.079556000
H	2.869266000	4.661683000	-0.687043000
H	1.953822000	4.539782000	1.631102000
H	1.149073000	2.354195000	2.504756000
H	1.362083000	-2.597753000	2.151814000
H	2.352610000	-4.548563000	0.980204000
H	3.248276000	-4.263421000	-1.331744000
H	3.191943000	-2.060698000	-2.413695000
H	1.761510000	1.186102000	-3.174118000
H	3.331668000	0.345731000	-3.169174000
H	1.810644000	-0.571503000	-3.296296000
H	-3.089856000	2.043600000	-0.906368000
H	-5.506395000	2.184708000	-0.429716000
H	-6.790170000	0.129570000	0.128974000
H	-5.623570000	-2.064345000	0.226401000
H	-3.205034000	-2.202877000	-0.224939000
H	-0.387882000	-0.482347000	3.354454000
H	-0.880673000	-1.610701000	-0.941945000



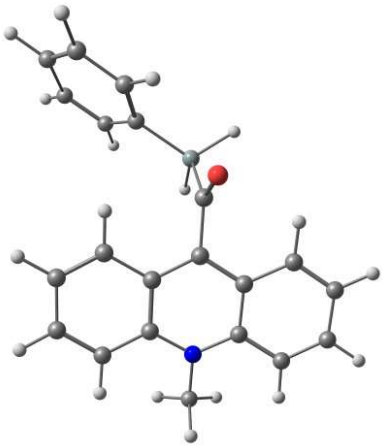
R = AsH			
Structure no. 4			
E = –2466.02342961 Ha			
Atom	X	Y	Z
C	0.161862000	-2.508448000	0.000000000
C	-0.591265000	-1.338574000	0.000000000
C	0.000000000	-0.045559000	0.000000000
C	1.422826000	-0.043876000	0.000000000
C	2.178375000	-1.210035000	0.000000000
C	1.562446000	-2.470064000	0.000000000
As	-0.951503000	1.612964000	0.000000000
H	1.938837000	0.915763000	0.000000000
H	-1.676677000	-1.412612000	0.000000000
H	3.266731000	-1.139833000	0.000000000
H	2.151144000	-3.384640000	0.000000000
H	-0.351769000	-3.470758000	0.000000000
H	-2.334120000	0.963613000	0.000000000



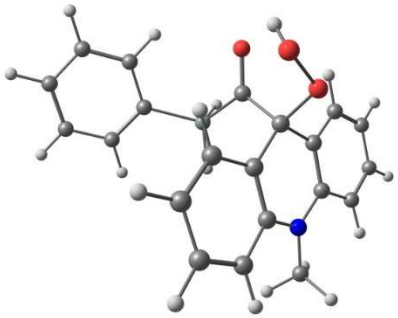
R = AsH			
Structure no. 6 *E* = −3250.06294234 Ha			
Atom	X	Y	Z
C	0.702670000	0.821614000	-0.128643000
C	0.337936000	-0.076496000	0.887204000
C	1.355638000	-0.663752000	1.654154000
C	2.692946000	-0.341960000	1.418354000
C	3.041195000	0.554688000	0.411477000
C	2.037446000	1.134166000	-0.369149000
As	-1.549133000	-0.582512000	1.057270000
C	-1.746572000	-0.412126000	3.023991000
O	-0.851095000	-0.730986000	3.783195000
C	-3.139971000	-0.052434000	3.673339000
C	-3.761045000	1.190285000	3.060052000
C	-4.532437000	1.075782000	1.884138000
N	-4.742586000	-0.203419000	1.324030000
C	-4.758402000	-1.324802000	2.179528000
C	-4.016520000	-1.275481000	3.376868000
C	-5.059254000	2.229875000	1.295525000
C	-4.818076000	3.482823000	1.866295000
C	-4.067620000	3.597284000	3.032378000
C	-3.549610000	2.443398000	3.627258000
C	-5.494697000	-2.474782000	1.874373000
C	-5.480916000	-3.566789000	2.744527000
C	-4.755371000	-3.518828000	3.932554000
C	-4.028603000	-2.367312000	4.241345000
O	-2.926800000	0.114121000	5.051415000
C	-5.199981000	-0.333591000	-0.048220000
H	-6.100907000	-2.518071000	0.976788000
H	-6.059521000	-4.450165000	2.490446000
H	-4.751853000	-4.365224000	4.611682000
H	-3.462753000	-2.294359000	5.163207000
H	-2.977534000	2.497710000	4.546753000
H	-3.885379000	4.569670000	3.478531000
H	-5.238443000	4.366140000	1.394222000
H	-5.681758000	2.161142000	0.410744000
H	-4.870507000	-1.297840000	-0.441938000
H	-6.291723000	-0.263590000	-0.155768000
H	-4.740956000	0.451726000	-0.652861000
H	-0.069862000	1.282662000	-0.740709000
H	2.291912000	1.834582000	-1.158910000
H	4.084465000	0.800030000	0.236333000
H	3.466359000	-0.799964000	2.029627000
H	1.099341000	-1.355464000	2.446150000
H	-1.998917000	-0.158207000	5.209278000
H	-2.059833000	0.842622000	0.844020000



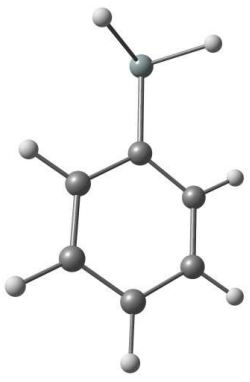
R = SiH_2			
Structure no. 1 *E* = –1230.35595605 Ha			
Atom	X	Y	Z
C	-3.914392000	-0.991816000	-0.743446000
C	-3.305857000	-0.796389000	0.512611000
C	-3.957589000	0.015727000	1.459986000
C	-5.186829000	0.606095000	1.165215000
C	-5.777761000	0.400994000	-0.082559000
C	-5.140285000	-0.395645000	-1.036802000
Si	-1.678270000	-1.606506000	0.933357000
C	-0.442517000	-1.262983000	-0.546332000
O	-0.665983000	-1.749053000	-1.643082000
C	0.804601000	-0.408165000	-0.353231000
C	2.054485000	-1.027774000	-0.169166000
C	3.201997000	-0.215652000	0.131530000
N	3.053343000	1.150734000	0.256035000
C	1.866063000	1.783511000	-0.051403000
C	0.700412000	0.994382000	-0.340370000
C	2.216769000	-2.443328000	-0.274075000
C	3.445654000	-3.026050000	-0.104342000
C	4.570777000	-2.213627000	0.168203000
C	4.461625000	-0.843836000	0.285007000
C	1.762337000	3.194877000	-0.097087000
C	0.552799000	3.791036000	-0.386554000
C	-0.608416000	3.025703000	-0.642895000
C	-0.532365000	1.657015000	-0.626408000
C	4.195550000	1.955772000	0.736906000
H	5.357263000	-0.264248000	0.458075000
H	5.548081000	-2.672865000	0.276709000
H	3.561840000	-4.100188000	-0.194492000
H	1.354334000	-3.050276000	-0.521212000
H	-1.409866000	1.061548000	-0.852618000
H	-1.546093000	3.521087000	-0.867941000
H	0.499501000	4.874142000	-0.429696000
H	2.628192000	3.823684000	0.054046000
H	4.778224000	1.366913000	1.440367000
H	4.828345000	2.275445000	-0.095325000
H	3.823172000	2.823700000	1.273777000
H	-3.510064000	0.182855000	2.436280000
H	-5.682752000	1.222671000	1.908619000
H	-6.735150000	0.859251000	-0.311258000
H	-5.600833000	-0.557023000	-2.006611000
H	-3.429562000	-1.609060000	-1.495045000
H	-1.106794000	-1.040924000	2.181886000
H	-1.709925000	-3.087433000	1.001100000



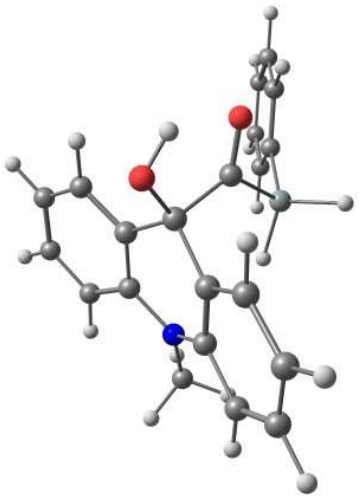
R = SiH_2			
Structure no. 2			
E = –1381.51829108 Ha			
Atom	X	Y	Z
C	3.552791000	0.394276000	-1.670953000
C	2.968372000	-0.666593000	-0.957021000
C	3.776633000	-1.393390000	-0.062430000
C	5.123332000	-1.072487000	0.105346000
C	5.688170000	-0.019573000	-0.617596000
C	4.901173000	0.714553000	-1.505453000
Si	1.159996000	-1.101017000	-1.204884000
C	0.324835000	-1.299394000	0.542611000
O	0.794739000	-2.144421000	1.297339000
C	-0.905216000	-0.453829000	0.954827000
C	-0.606984000	1.025228000	0.813560000
C	-1.426212000	1.873722000	0.032887000
N	-2.454466000	1.352597000	-0.765725000
C	-2.832724000	0.012052000	-0.666756000
C	-2.076316000	-0.899423000	0.102273000
C	-1.176308000	3.260259000	0.060689000
C	-0.102813000	3.781321000	0.775708000
C	0.748683000	2.939631000	1.487528000
C	0.481858000	1.573719000	1.504905000
C	-3.980987000	-0.472945000	-1.328257000
C	-4.330100000	-1.817255000	-1.266902000
C	-3.561369000	-2.723334000	-0.535805000
C	-2.450284000	-2.249297000	0.151277000
O	-1.351208000	-0.819182000	2.288012000
O	-0.286875000	-0.651055000	3.266325000
C	-3.083296000	2.202685000	-1.769492000
H	-4.626056000	0.205117000	-1.871399000
H	-5.221041000	-2.152687000	-1.789865000
H	-3.833455000	-3.772174000	-0.485893000
H	-1.858856000	-2.922514000	0.762797000
H	1.102319000	0.911420000	2.094892000
H	1.596082000	3.337974000	2.035346000
H	0.061303000	4.855002000	0.772581000
H	-1.833355000	3.944850000	-0.459828000
H	-3.384357000	1.598083000	-2.625085000
H	-3.963728000	2.735119000	-1.386603000
H	-2.361754000	2.934799000	-2.132779000
H	2.950232000	0.979537000	-2.360941000
H	5.335158000	1.537162000	-2.066761000
H	6.737587000	0.229008000	-0.486905000
H	5.732266000	-1.643067000	0.800865000
H	3.344888000	-2.205787000	0.515310000
H	0.216853000	-1.467296000	3.079875000
H	0.502142000	-0.067942000	-2.042867000
H	0.992422000	-2.432838000	-1.843365000



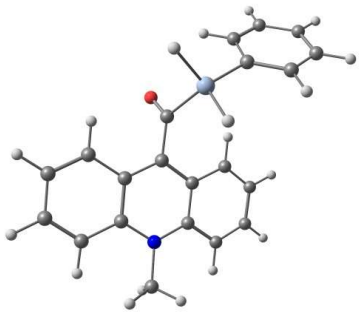
R = SiH_2			
Structure no. 4			
E = –522.347264664 Ha			
Atom	X	Y	Z
C	-1.621157000	1.201266000	-0.000191000
C	-0.225884000	1.192996000	0.010062000
C	0.533209000	-0.000224000	0.019042000
C	-0.226195000	-1.193194000	0.010053000
C	-1.621501000	-1.201074000	-0.000191000
C	-2.337746000	0.000181000	-0.004083000
Si	2.475279000	-0.000031000	-0.139700000
H	0.299508000	-2.147724000	0.018427000
H	0.300134000	2.147345000	0.018451000
H	-2.157393000	-2.150629000	0.001746000
H	-3.426090000	0.000339000	-0.010215000
H	-2.156817000	2.150953000	0.001742000
H	2.740939000	1.141328000	0.858528000
H	2.741453000	-1.140886000	0.858965000



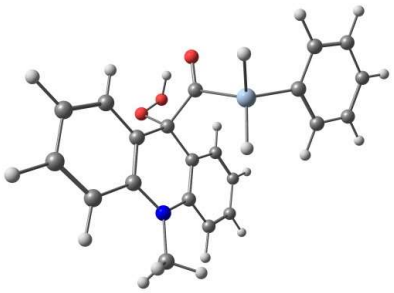
R = SiH_2			
Structure no. 6 *E* = –1306.39547985 Ha			
Atom	X	Y	Z
C	0.031585000	1.849429000	-2.012449000
C	0.742633000	1.139757000	-1.042057000
C	1.142796000	1.789437000	0.145528000
C	0.820783000	3.149945000	0.311111000
C	0.097338000	3.832964000	-0.662776000
C	-0.303687000	3.188666000	-1.832674000
C	1.058679000	-0.332220000	-1.278667000
C	2.217027000	-0.785558000	-0.399215000
C	2.566475000	-0.074314000	0.769337000
N	1.864278000	1.087841000	1.123581000
C	3.638915000	-0.546302000	1.549924000
C	4.322586000	-1.705380000	1.192937000
C	3.973960000	-2.409938000	0.041065000
C	2.928999000	-1.935744000	-0.747476000
C	-0.207002000	-1.175620000	-0.911184000
O	-0.722850000	-1.835974000	-1.807618000
O	1.334091000	-0.577205000	-2.641196000
C	2.050915000	1.671468000	2.441362000
Si	-1.028795000	-1.300597000	0.840478000
C	-2.852021000	-0.886219000	0.686943000
C	-3.654323000	-1.434813000	-0.331263000
C	-5.012424000	-1.128740000	-0.412313000
C	-5.595327000	-0.270093000	0.522191000
C	-4.814834000	0.286108000	1.535918000
C	-3.455095000	-0.018396000	1.614757000
H	3.964064000	0.006119000	2.422813000
H	5.145109000	-2.045729000	1.815385000
H	4.511163000	-3.309004000	-0.242879000
H	2.654600000	-2.443287000	-1.665901000
H	-0.239273000	1.330057000	-2.925208000
H	-0.861838000	3.721483000	-2.595595000
H	-0.137025000	4.882129000	-0.507355000
H	1.160876000	3.688904000	1.186765000
H	2.185284000	0.874116000	3.174146000
H	2.914910000	2.349232000	2.498573000
H	1.154245000	2.227134000	2.720567000
H	-2.858254000	0.428307000	2.406105000
H	-5.262363000	0.958624000	2.262231000
H	-6.653595000	-0.033249000	0.457926000
H	-5.616382000	-1.559338000	-1.205972000
H	-3.209031000	-2.092668000	-1.071767000
H	0.628828000	-1.189158000	-2.932566000
H	-0.807396000	-2.716150000	1.237018000
H	-0.398530000	-0.405235000	1.838468000



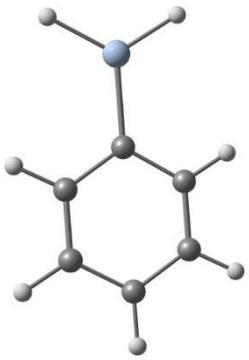
R = GeH_2			
Structure no. 1 *E* = –3015.85885833 Ha			
Atom	X	Y	Z
C	-3.847288000	-0.587864000	-1.046257000
C	-3.253335000	0.470485000	-0.342128000
C	-3.888103000	0.972882000	0.804878000
C	-5.093594000	0.423602000	1.239024000
C	-5.679015000	-0.627972000	0.529805000
C	-5.055225000	-1.134506000	-0.611513000
Ge	-1.609175000	1.248350000	-0.965583000
C	-0.284296000	1.127133000	0.544690000
O	-0.504047000	1.741629000	1.571274000
C	0.988608000	0.315874000	0.387179000
C	0.925362000	-1.088732000	0.328618000
C	2.124481000	-1.836165000	0.071598000
N	3.305532000	-1.162235000	-0.164338000
C	3.407196000	0.205386000	-0.008528000
C	2.223733000	0.978459000	0.256010000
C	2.060893000	-3.251073000	0.076026000
C	0.857691000	-3.889107000	0.291700000
C	-0.336218000	-3.163402000	0.510886000
C	-0.300116000	-1.793289000	0.535574000
C	4.653688000	0.871620000	-0.091528000
C	4.716593000	2.241920000	0.049398000
C	3.555378000	3.017336000	0.274027000
C	2.337584000	2.397683000	0.379372000
C	4.493318000	-1.923781000	-0.604342000
H	5.572989000	0.320841000	-0.230548000
H	5.683892000	2.730893000	-0.005835000
H	3.634232000	4.093757000	0.376493000
H	1.445077000	2.976400000	0.579774000
H	-1.206620000	-1.233698000	0.739057000
H	-1.268825000	-3.690790000	0.676699000
H	0.833999000	-4.974028000	0.303513000
H	2.951187000	-3.850443000	-0.050765000
H	5.093778000	-1.302685000	-1.263607000
H	5.092059000	-2.245910000	0.251786000
H	4.173675000	-2.788418000	-1.179116000
H	-3.365970000	-0.986836000	-1.935206000
H	-5.512067000	-1.948560000	-1.165886000
H	-6.620962000	-1.050409000	0.865932000
H	-5.579066000	0.818520000	2.125999000
H	-3.437038000	1.788560000	1.362666000
H	-1.058596000	0.489471000	-2.180848000
H	-1.688498000	2.749829000	-1.238225000



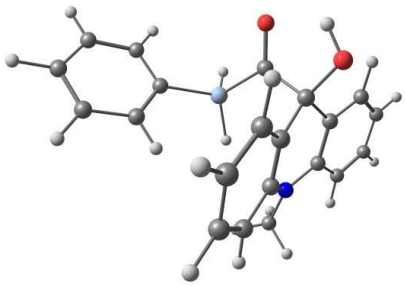
R = GeH_2			
Structure no. 2			
E = –3167.02306322 Ha			
Atom	X	Y	Z
C	3.234267000	0.700190000	-0.958299000
C	2.840763000	-0.630274000	-0.755987000
C	3.814541000	-1.571731000	-0.393361000
C	5.146474000	-1.191689000	-0.228165000
C	5.525215000	0.136046000	-0.433411000
C	4.566403000	1.082416000	-0.798678000
Ge	0.995021000	-1.159116000	-0.969150000
C	0.128941000	-1.218586000	0.830914000
O	0.547978000	-2.014179000	1.655023000
C	-1.058453000	-0.275145000	1.118093000
C	-2.214381000	-0.747480000	0.260027000
C	-2.872299000	0.108862000	-0.649079000
N	-2.406461000	1.405725000	-0.877982000
C	-1.383428000	1.954509000	-0.092532000
C	-0.661061000	1.158474000	0.826797000
C	-4.014230000	-0.384033000	-1.315198000
C	-4.444822000	-1.692556000	-1.127336000
C	-3.766255000	-2.551561000	-0.262328000
C	-2.664662000	-2.063496000	0.429997000
C	-1.041467000	3.316405000	-0.214621000
C	0.032355000	3.852040000	0.488975000
C	0.792999000	3.050767000	1.337914000
C	0.433749000	1.716015000	1.501365000
O	-1.564737000	-0.474175000	2.461596000
O	-0.513012000	-0.285944000	3.450159000
C	-2.927769000	2.165134000	-2.008491000
H	-4.589835000	0.262443000	-1.964600000
H	-5.327515000	-2.036289000	-1.658745000
H	-4.099988000	-3.573236000	-0.116199000
H	-2.142048000	-2.695942000	1.139785000
H	0.983402000	1.091052000	2.193515000
H	1.640654000	3.458656000	1.878226000
H	0.268300000	4.905469000	0.368982000
H	-1.626831000	3.972813000	-0.845205000
H	-3.223593000	1.480902000	-2.803692000
H	-3.789884000	2.789951000	-1.741247000
H	-2.142851000	2.804858000	-2.412252000
H	3.532146000	-2.608175000	-0.229674000
H	5.889714000	-1.931313000	0.055500000
H	6.563068000	0.431835000	-0.309486000
H	4.855880000	2.116925000	-0.960024000
H	2.492725000	1.444789000	-1.234802000
H	-0.058233000	-1.145726000	3.354316000
H	0.280164000	-0.211480000	-1.939752000
H	0.936146000	-2.597329000	-1.489781000



R = GeH_2			
Structure no. 4			
E = –2307.81227692 Ha			
Atom	X	Y	Z
C	-1.199266000	2.198439000	0.000000000
C	-1.202870000	0.811348000	0.000000000
C	0.000000000	0.044739000	0.000000000
C	1.203486000	0.810261000	0.000000000
C	1.201066000	2.197392000	0.000000000
C	0.001250000	2.927799000	0.000000000
Ge	-0.000765000	-1.836885000	0.000000000
H	2.157388000	0.285396000	0.000000000
H	-2.157214000	0.287284000	0.000000000
H	2.154308000	2.727648000	0.000000000
H	0.001747000	4.014926000	0.000000000
H	-2.152034000	2.729534000	0.000000000
H	1.314956000	-2.602332000	0.000000000
H	-1.316670000	-2.601999000	0.000000000



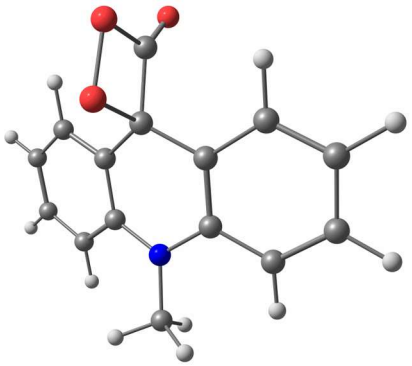
R = GeH_2			
Structure no. 6 *E* = –3091.89958062 Ha			
Atom	X	Y	Z
C	3.012001000	0.506171000	-0.620313000
C	2.649671000	-0.846486000	-0.541766000
C	3.653988000	-1.801698000	-0.333894000
C	4.988035000	-1.415304000	-0.200642000
C	5.335927000	-0.066346000	-0.280555000
C	4.345121000	0.894769000	-0.490463000
Ge	0.805763000	-1.393181000	-0.720555000
C	-0.079161000	-1.181419000	1.053458000
O	0.308982000	-1.904258000	1.956210000
C	-1.188870000	-0.130726000	1.370939000
C	-0.645939000	1.247071000	1.019012000
C	-0.934831000	1.844584000	-0.227467000
N	-1.773817000	1.195089000	-1.143164000
C	-2.650857000	0.193494000	-0.698857000
C	-2.411482000	-0.465092000	0.525871000
C	-0.376774000	3.105402000	-0.516051000
C	0.460886000	3.738346000	0.399417000
C	0.747888000	3.145033000	1.628799000
C	0.184924000	1.906803000	1.926758000
C	-3.788935000	-0.163006000	-1.446097000
C	-4.644408000	-1.167538000	-1.001498000
C	-4.402281000	-1.824430000	0.204731000
C	-3.290569000	-1.459605000	0.959437000
O	-1.476604000	-0.232024000	2.748352000
C	-1.831645000	1.651272000	-2.522045000
H	-4.026218000	0.362434000	-2.363075000
H	-5.514604000	-1.422845000	-1.599245000
H	-5.071701000	-2.603058000	0.555610000
H	-3.092439000	-1.931566000	1.915625000
H	0.369283000	1.431177000	2.883851000
H	1.394912000	3.640125000	2.345453000
H	0.874686000	4.711386000	0.150656000
H	-0.622057000	3.611315000	-1.441828000
H	-2.103389000	0.814444000	-3.167394000
H	-2.552612000	2.465681000	-2.681237000
H	-0.842816000	1.996183000	-2.829907000
H	2.248014000	1.262886000	-0.778349000
H	4.610173000	1.946366000	-0.552413000
H	6.374599000	0.235337000	-0.179610000
H	5.756313000	-2.165873000	-0.038305000
H	3.395854000	-2.855156000	-0.269188000
H	-0.902643000	-0.953931000	3.072699000
H	0.116485000	-0.614496000	-1.842092000
H	0.765319000	-2.891757000	-1.010498000



Structure no. 3

E = –858.562621852 Ha

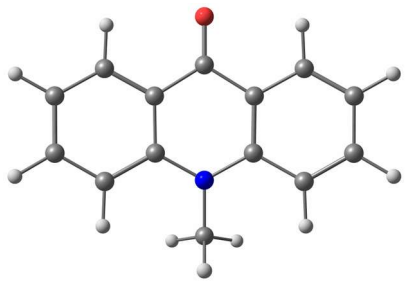
Atom	X	Y	Z
C	0.000001668	0.000001693	-0.000001706
C	-0.000001089	-0.000001851	0.000001165
C	-0.000000367	-0.000001169	-0.000000734
C	-0.000002814	0.000000924	0.000001399
C	-0.000000362	0.000001022	-0.000004683
C	0.000002700	0.000001164	0.000003988
H	-0.000002124	-0.000001075	-0.000000977
H	-0.000000648	-0.000000525	0.000000174
H	-0.000000321	-0.000000268	-0.000000218
H	-0.000000691	0.000002504	0.000001310
C	-0.000017086	0.000054670	0.000000418
C	0.000010024	-0.000005601	0.000004297
C	0.000000008	0.000002454	0.000003356
N	0.000000508	-0.000004494	-0.000002943
C	0.000010417	-0.000023592	-0.000005269
C	0.000002427	0.000000477	0.000001251
C	-0.000002474	0.000002539	-0.000002411
C	0.000001761	0.000000169	-0.000000460
C	-0.000000665	-0.000000821	0.000001710
C	-0.000000299	-0.000001818	-0.000000104
H	-0.000000966	0.000001462	-0.000000044
H	-0.000000352	0.000000638	0.000000331
H	-0.000000532	-0.000000897	0.000000546
H	-0.000000829	-0.000002301	0.000003179
H	0.000001748	-0.000002958	0.000000892
H	-0.000001643	-0.000002553	-0.000000051
H	-0.000000226	-0.000002195	-0.000003133
O	-0.000004137	0.000004980	0.000005157
O	-0.000005940	0.000022784	0.000000099
O	0.000012303	-0.000045363	-0.000006540



Structure no. 5

E = –670.130875334 Ha

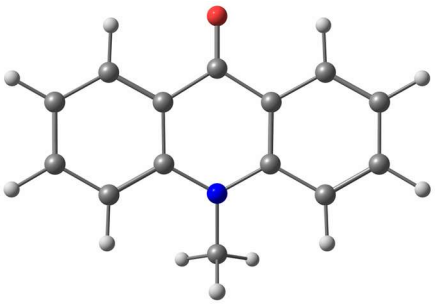
Atom	X	Y	Z
C	-0.000001670	-0.000000453	-0.000001193
C	0.000008374	-0.000005822	-0.000001257
C	0.000002869	0.000003676	-0.000003162
C	-0.000004216	0.000000572	0.000006893
C	-0.000005048	0.000000891	-0.000003333
C	0.000004889	-0.000001754	-0.000002000
N	-0.000012637	0.000017666	-0.000007600
C	0.000006051	-0.000000082	0.000013394
C	-0.000000121	0.000000061	-0.000000647
C	0.000007382	-0.000003957	0.000003724
C	0.000002584	0.000000596	-0.000005419
C	-0.000003789	-0.000000740	-0.000003533
C	0.000000399	0.000001187	0.000002142
C	-0.000007344	-0.000001750	0.000004438
O	-0.000006036	0.000000369	-0.000002764
H	0.000004494	-0.000002110	-0.000007293
H	0.000001227	-0.000000156	0.000000932
H	0.000001465	0.000000453	0.000000462
H	-0.000001085	0.000000180	0.000002749
H	0.000001397	0.000000188	-0.000001976
H	0.000001000	0.000000064	0.000001035
H	0.000000113	0.000000643	0.000000580
H	-0.000002946	-0.000001652	0.000004237
C	0.000015838	-0.000020655	0.000006897
H	-0.000003439	0.000010208	-0.000003254
H	-0.000003390	0.000004209	-0.000004274
H	-0.000006362	-0.000001834	0.000000222



Structure no. 5*

E = –669.953518683 Ha

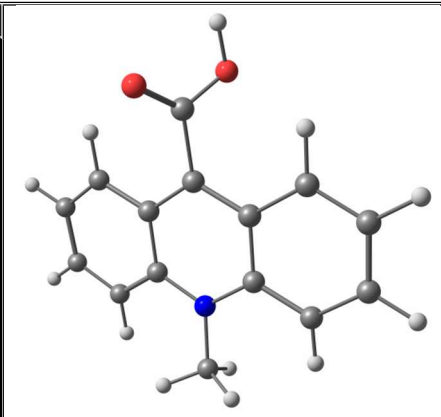
Atom	X	Y	Z
C	0.001468800	0.001306003	-0.014311619
C	0.004149509	-0.000735113	0.018325511
C	-0.007929979	0.000236431	0.003322763
C	0.006366228	-0.000302096	-0.001943657
C	0.002246243	-0.000461559	0.001194686
C	-0.005244037	-0.001119324	-0.002114223
C	0.002234971	0.002222086	0.001039014
C	-0.001297352	-0.000930055	-0.008452168
C	0.017660061	-0.003111007	-0.005658745
N	-0.006147717	-0.003163889	-0.003149872
C	0.001646542	0.000527929	0.006435157
C	0.002147453	-0.000444212	0.001369963
C	-0.004625234	-0.001228109	-0.003212401
C	-0.011272831	0.003546751	0.008307965
C	0.002077794	0.004103694	0.000763843
O	-0.002882271	-0.000726284	-0.001551682
H	0.000157316	0.000901467	0.000726183
H	0.000013596	-0.000065916	0.000470644
H	0.000088075	0.000455664	0.000087984
H	-0.000411324	0.000239363	0.000014109
H	-0.000182535	0.000199133	-0.000392060
H	0.000158968	0.000443207	-0.000037869
H	0.000401083	-0.000134057	-0.000217245
H	0.000774354	0.000792950	-0.000369232
H	-0.000473261	-0.000738933	0.000646528
H	0.000239722	-0.000864334	-0.000619243
H	-0.001364177	-0.000949789	-0.000674335



Structure no. 7

E = –783.845241706 Ha

Atom	X	Y	Z
C	-0.000003697	0.000002446	-0.000014793
C	0.000002314	-0.000000933	0.000008333
C	-0.000001217	-0.000003198	0.000002700
C	0.000004336	0.000000328	0.000001581
C	0.000004926	-0.000001305	0.000003524
C	-0.000007755	-0.000001029	-0.000007555
N	0.000007393	0.000000704	0.000000979
C	-0.000005213	-0.000002967	-0.000001330
C	0.000000330	0.000003971	0.000003834
C	-0.000011000	-0.000008618	-0.000007880
C	-0.000002247	0.000003865	-0.000007202
C	-0.000002250	0.000001186	0.000006776
C	0.000003876	0.000000304	0.000005644
C	0.000009818	0.000004769	-0.000005549
C	-0.000012508	0.000004987	0.000019564
O	0.000003593	0.000002240	0.000001128
C	-0.000008468	-0.000005079	-0.000006976
O	-0.000006529	-0.000007501	-0.000010075
H	0.000001778	0.000001712	0.000001095
H	-0.000000735	0.000001005	0.000000100
H	0.000002823	0.000000808	0.000000856
H	0.000009003	0.000001827	-0.000001928
H	0.000001635	0.000000603	0.000003297
H	0.000001306	-0.000000319	0.000001102
H	-0.000001737	-0.000001334	-0.000000322
H	-0.000001556	-0.000001767	-0.000002097
H	0.000002183	0.000002078	-0.000006761
H	-0.000000947	-0.000001576	0.000003175
H	0.000002443	0.000002699	-0.000000949
H	0.000008102	0.000000095	0.000009727



Structure CO_2

E = –188.580938479 Ha

Atom	X	Y	Z
C	-0.000683228	-0.000000000	-0.000001192
O	0.000341891	0.000000000	-0.000158006
O	0.000341337	0.000000000	0.000159199

Structure H_2O

E = –76.4197366208 Ha

Atom	X	Y	Z
O	-0.000092754	0.000000000	-0.000065587
H	0.000031598	0.000000000	0.000053695
H	0.000061157	-0.000000000	0.000011892

Structure OH^-

E = –75.7262923857 Ha

Atom	X	Y	Z
O	0.000000000	0.000000000	0.000008875
H	0.000000000	0.000000000	-0.000008875

Structure OOH^-

E = –75.7262923857 Ha

Atom	X	Y	Z
O	0.000158315	0.000000000	-0.000030230
O	-0.000018291	-0.000000000	0.000013673
H	-0.000140024	-0.000000000	0.000016557