Improving phase-transfer catalysis by enhancing non-covalent interactions

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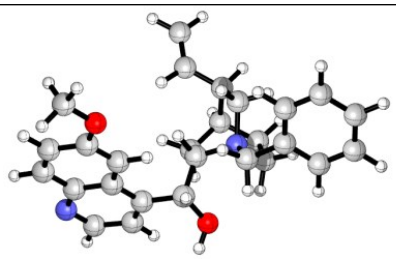
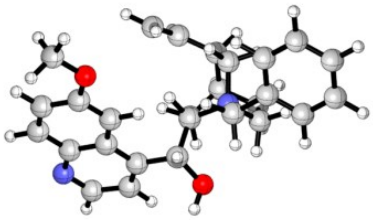
Figure S1. Optimised geometries of all different conformers of the catalyst under study at m062x/aug-cc-pVDZ computational level.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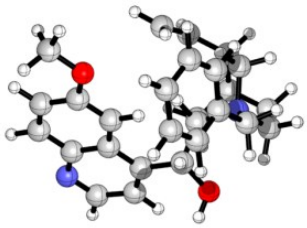	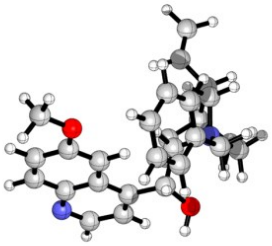
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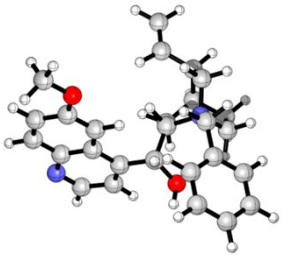	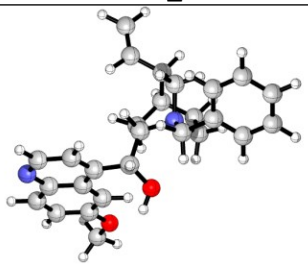
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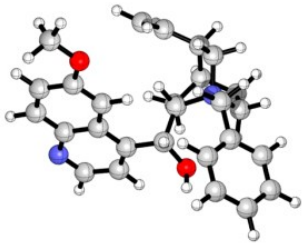	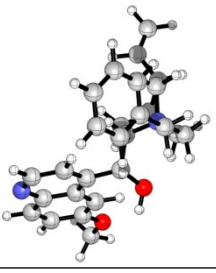
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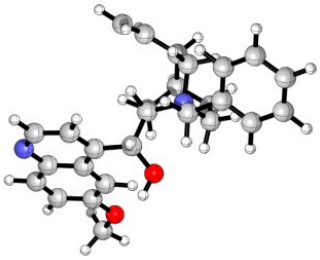	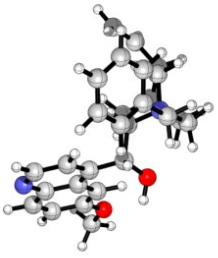
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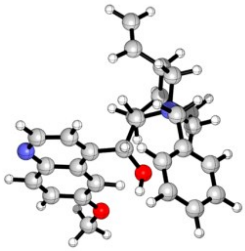
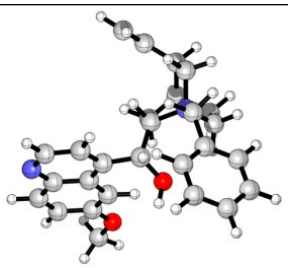
	
Conf_11	**Conf_12**

Figure S2. Graphical benchmark of the relative free energies (ΔG), kJ/mol, of all different conformers of the catalyst under study at m062x/aug-cc-pVTZ//aug-cc-pVDZ//6-31g(d) computational level.

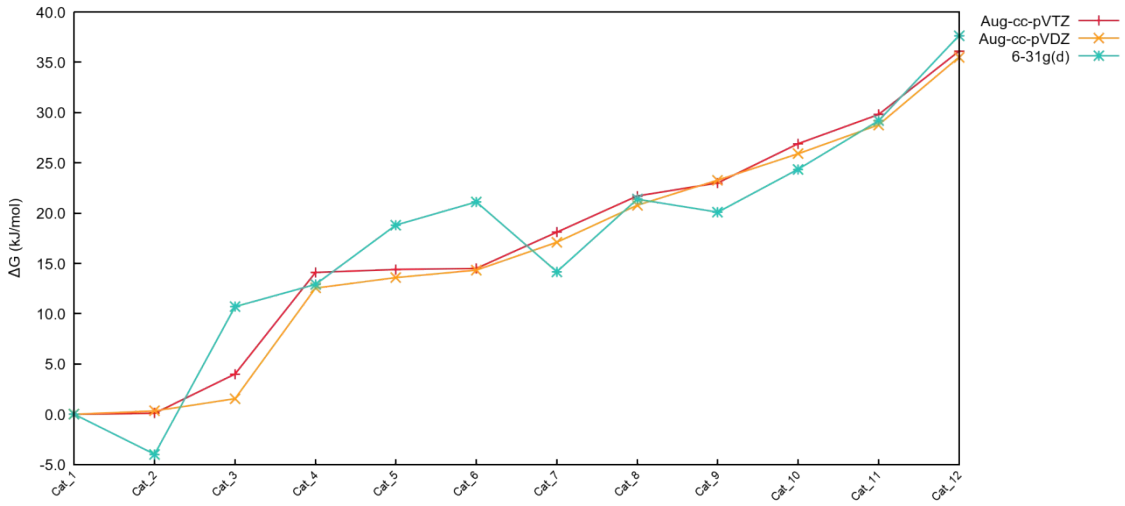


Table S1. Relative free energies (ΔG), kJ/mol, of all different conformers of the catalyst under study at m062x/aug-cc-pVDZ and m062x/6-31g(d) computational level.

Conformer	ΔG kJ/mol aug-cc-pVDZ	ΔG kJ/mol 6-31g(d)
Conf_1	0.00	0.00
Conf_2	0.33	-3.98
Conf_3	1.55	10.70
Conf_4	12.54	12.91
Conf_5	13.59	18.81
Conf_6	14.33	21.11
Conf_7	17.10	14.17
Conf_8	20.78	21.38
Conf_9	23.28	20.09
Conf_10	25.90	24.36
Conf_11	28.77	29.18
Conf_12	35.50	37.65

Table S2. Boltzmann distribution of the different conformers under study at m062x/aug-cc-pVTZ

Name	%
Cat_1	47.37
Cat_2	46.05
Cat_3	6.45
Cat_4	0.05
Cat_5	0.04
Cat_6	0.04
Cat_7	0.01
Cat_8	0.00
Cat_9	0.00
Cat_10	0.00
Cat_11	0.00
Cat_12	0.00

Table S3. Free interaction energies (ΔG, kJ mol^{-1}) calculated at m062x/aug-cc-pVDZ and m062x/6-31g(d) computational level.

Conformer	ΔG kJ/mol aug-cc-pVDZ	ΔG kJ/mol 6-31g(d)
complex_Cl_1	-151.52	-164.38
complex_Cl_2	-120.23	-132.81
complex_Cl_3	-103.39	-106.59
complex_Cl_5	-98.00	-101.17
complex_Br_1	-159.94	-188.15
complex_Br_2	-127.30	-165.98
complex_Br_3	-113.57	-129.35
complex_Br_4	-117.81	-
complex_Br_5	-108.14	-128.32
complex_$MeCO_2$_1	-176.91	-216.22
complex_$MeCO_2$_2	-141.46	-174.57
complex_$MeCO_2$_3	-113.46	-137.96
complex_CN_1	-145.96	-177.98
complex_NC_1	-142.38	-178.53
complex_CN_2	-112.83	-139.53
complex_CN_3	-78.94	-108.11

Figure S3. Graphical benchmark of the free energies (ΔG), kJ/mol, calculated at m062x/aug-cc-pVTZ//aug-cc-pVDZ//6-31g(d) computational level.

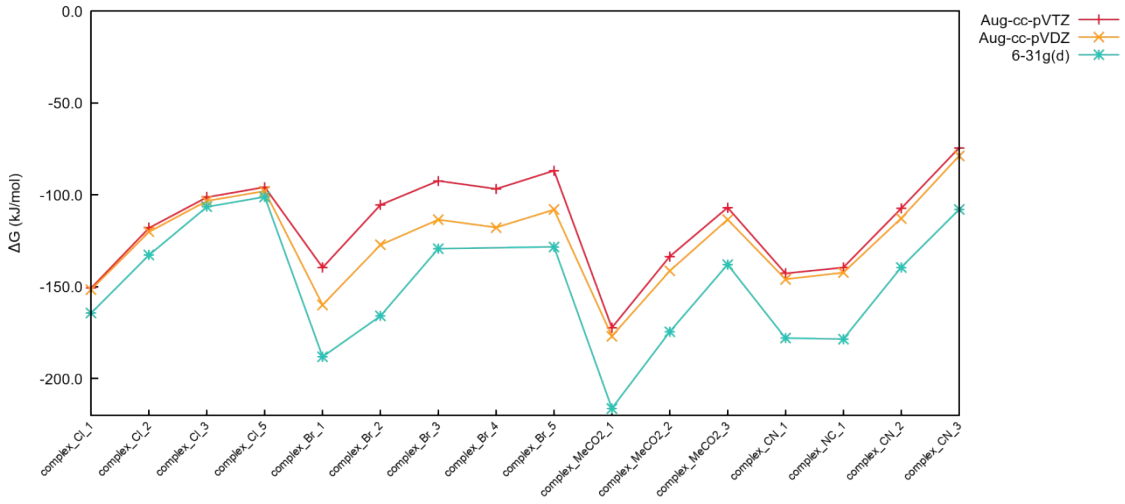


Table S4. Interaction distance (Å), electron density at the BCP (ρ) and Laplacian ($\nabla^2\rho$), for all the complexes studied at M062X/aug–cc–pVDZ computational level.

Name	Distance	ρ (BCP)	$\nabla^2\rho$(BCP)
complex_Cl_1	2.77	0.009	0.025
	2.56	0.014	0.037
	2.61	0.013	0.034
	2.05	0.035	0.090
complex_Cl_2	2.47	0.017	0.046
	2.78	0.010	0.025
	2.44	0.018	0.049
	2.62	0.012	0.033
	2.70	0.012	0.030
complex_Cl_3	2.76	0.010	0.029
	2.68	0.012	0.033
	2.44	0.017	0.049
complex_Cl_5	2.76	0.010	0.029
	2.68	0.012	0.033
	2.44	0.017	0.049
complex_Br_1	2.79	0.012	0.027
	2.91	0.009	0.022
	2.74	0.012	0.030
	2.26	0.028	0.064
	2.93	0.010	0.030
complex_Br_2	2.57	0.017	0.041
	2.70	0.014	0.032
	2.89	0.010	0.024
	2.85	0.010	0.025

	2.92	0.009	0.022
	3.80	0.004	0.012
	3.34	0.005	0.013
complex_Br_3	2.88	0.010	0.026
	2.91	0.010	0.025
	3.14	0.007	0.018
	2.64	0.015	0.036
complex_Br_4	2.71	0.013	0.036
	2.89	0.010	0.024
complex_Br_5	3.09	0.008	0.021
	2.71	0.014	0.038
	3.23	0.006	0.016
	3.42	0.004	0.011
complex_$MeCO_2$_1	1.49	0.079	0.148
	2.14	0.018	0.060
	2.26	0.014	0.045
	2.48	0.012	0.034
	2.28	0.015	0.043
complex_$MeCO_2$_2	2.31	0.015	0.041
	2.63	0.008	0.025
	2.05	0.022	0.075
	2.71	0.006	0.023
	2.18	0.017	0.054
	2.03	0.023	0.075
	2.80	0.006	0.021
complex_$MeCO_2$_3	2.18	0.018	0.057
	3.44	0.005	0.016
	2.46	0.011	0.037
	2.18	0.017	0.060
	2.21	0.017	0.053
complex_CN_1	2.65	0.008	0.023
	2.52	0.010	0.027
	1.68	0.052	0.140
	2.35	0.013	0.038
complex_NC_1	1.78	0.050	0.084
	2.44	0.012	0.033
	2.43	0.011	0.032
	2.75	0.009	0.025
complex_CN_2	2.23	0.018	0.052
	2.69	0.008	0.021
	2.30	0.015	0.044
	2.45	0.012	0.033
	2.37	0.012	0.036
complex_CN_3	2.67	0.008	0.025
	2.40	0.013	0.039
	2.17	0.019	0.059
	3.74	0.004	0.010

Figure S4. 2D-NCI plots of the interactions found for the most stable complex with each anion.

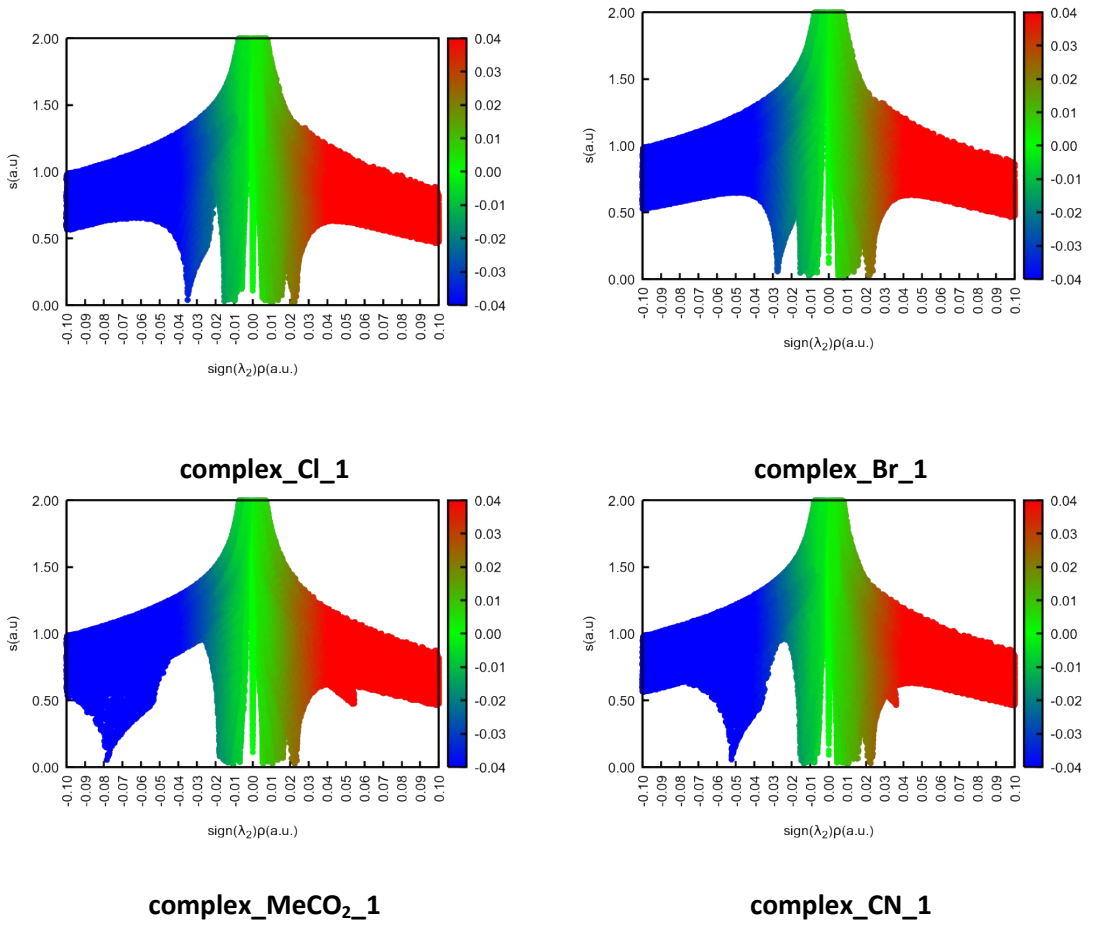
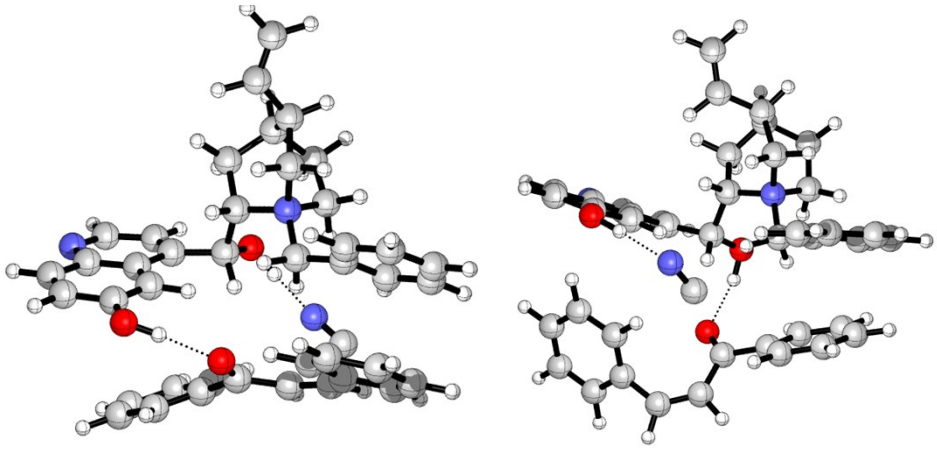


Table S5. NBO values of charge transfer energy E(2), in kJ/mol , from lone pairs of the corresponding anion to different σ*(X-C) antibonding orbital of the catalyst.

Name	Orb(1)	Orb(2)	E (2)
complex_Cl_1	LP(4)Cl63	σ*(1)O35-H36	124.432
complex_Cl_2	LP(4)Cl63	σ*(1)C16-H18	23.806
complex_Cl_3	LP(4)Cl63	σ*(1)C16-H17	31.421
complex_Cl_5	LP(4)Cl63	σ*(1)C16-N56	12.761
complex_Br_1	LP(4)Br63	σ*(1)O35-H36	92.382
complex_Br_2	LP(4)Br63	σ*(1)C16-H18	28.785
complex_Br_3	LP(4)Br63	σ*(1)C16-H17	24.56
complex_Br_4	LP(4)Br63	σ*(1)C7-H8	14.183
complex_Br_5	LP(4)Br63	σ*(1)C16-H17	10.501
complex_$MeCO_2$_1	LP(2)O64	σ*(1)O35-H36	251.667
complex_$MeCO_2$_2	LP(2)O65	σ*(1)C19-H20	27.447
complex_$MeCO_2$_3	LP(1)O65	σ*(1)C7-H8	12.217
complex_CN_1	LP(1)N64	σ*(1)O35-H36	184.974
complex_NC_1	LP(1)C64	σ*(1)O35-H36	258.32

complex_CN_2	LP(1)N64	σ*(1)C19-H20	27.237
complex_CN_3	LP(1)N64	σ*(1)C16-H17	36.693

Figure S5. Optimised geometries corresponding to the pre-TS of the two different CN^- possible interactions.



ΔΔG = 0.0 kJ/mol **ΔΔG = 26.2 kJ/mol**

Figure S6. Theoretical ee% for both reactions under study. On the left under the presence of **cat1**, on the right under the presence of **cat2**.

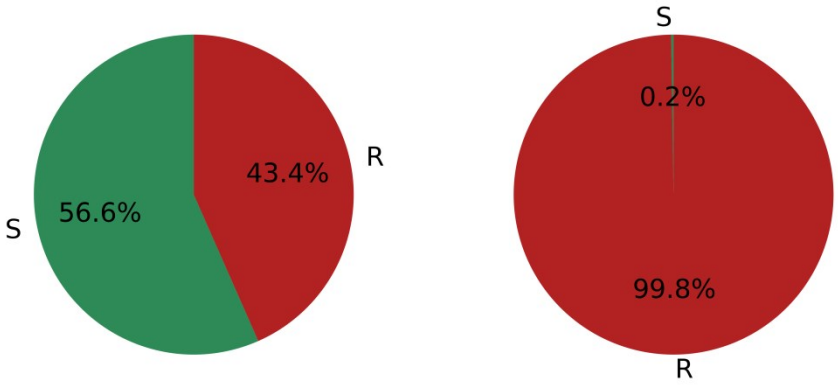


Table S6. Molecular graphs (AIM) and optimized geometries (Cartesian Coordinates in Å) for all the complexes under study. Green dots indicate bond critical (BCP)

Compound	Coordinates			
	Atom	x	y	z
conf_1	C	-0.139444	-0.912756	-0.032813
Img. freq. = 0	C	-1.093330	-2.495876	1.652914
SCF Energy (a.u.) = -1307.24374351	C	0.090829	-2.231408	0.720344
	H	0.292400	-0.079650	0.530739
	H	0.192888	-3.055342	0.004212
	H	1.031873	-2.153467	1.272696
	C	-2.451810	-1.849208	-0.337808
	H	-3.485279	-1.513100	-0.440642
	H	-2.088095	-2.215891	-1.297663
	C	-2.296731	-2.882424	0.790631
	H	-3.205527	-2.920228	1.401715
	H	-2.147302	-3.872603	0.348086
	H	-0.850885	-3.291328	2.363491
	C	-1.456364	-1.209390	2.420435
	H	-2.287584	-1.444186	3.095669
	C	-1.976770	-0.179962	1.386999
	H	-3.063986	-0.087887	1.428025
	H	-1.531943	0.810984	1.527285
	C	-1.960281	0.494989	-1.010772
	H	-1.229143	1.286221	-0.813196
	H	-1.782715	0.063030	-1.999515
	C	-3.359959	1.047114	-0.926571
	C	-4.379077	0.515690	-1.724228
	C	-3.644566	2.132133	-0.089916
	C	-5.669232	1.039500	-1.664380
	H	-4.158689	-0.304973	-2.407654
	C	-4.933310	2.657264	-0.028391
	H	-2.851682	2.574439	0.513728
	C	-5.948751	2.106736	-0.811258
	H	-6.454611	0.620767	-2.291316
	H	-5.145161	3.502381	0.624529
	H	-6.955557	2.519346	-0.766926
	C	0.525563	-0.872869	-1.418542
	H	0.381599	0.120132	-1.865032
	O	-0.079023	-1.858375	-2.233028
	H	0.377972	-1.879706	-3.084114
	C	2.017658	-1.088320	-1.232723
	C	2.853961	-0.029403	-0.753033
	C	2.591456	-2.306602	-1.493234
	C	2.392535	1.279888	-0.474085
	C	4.231994	-0.332831	-0.551383
	C	3.982220	-2.492684	-1.272027
	H	1.993872	-3.141314	-1.854108

	C	3.255873	2.247648	0.003913
	H	1.358345	1.573046	-0.643524
	C	5.092553	0.680341	-0.059872
	H	4.433806	-3.463657	-1.480782
	C	4.626708	1.941564	0.219551
	H	6.140709	0.425634	0.087638
	H	5.313159	2.696081	0.593382
	O	2.718972	3.468040	0.240086
	C	3.577835	4.489071	0.735859
	H	2.949966	5.375683	0.848890
	H	3.997099	4.210263	1.711945
	H	4.387072	4.703105	0.025210
	N	-1.642267	-0.610816	-0.023211
	C	-0.323260	-0.673512	3.253795
	H	0.569822	-0.320506	2.730146
	C	-0.354700	-0.616290	4.584319
	H	0.488934	-0.234019	5.156363
	H	-1.226971	-0.953394	5.146235
	N	4.774612	-1.557412	-0.812262

Compound	Coordinates			
	Atom	x	y	z
conf_2	C	-0.131956	-1.024920	0.056553
Img. freq. = 0	C	-1.083977	-2.517398	1.814746
SCF Energy (a.u.) = -1307.24448174	C	0.092769	-2.314864	0.858922
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	H	0.179965	-3.170108	0.179282
	H	1.037816	-2.213750	1.400653
	C	-2.458807	-1.932525	-0.185139
	H	-3.489237	-1.589014	-0.294073
	H	-2.106061	-2.342698	-1.132006
	C	-2.306504	-2.917000	0.986855
	H	-3.207820	-2.911805	1.610349
	H	-2.180961	-3.928316	0.587048
	H	-0.848762	-3.287921	2.555443
	C	-1.395068	-1.183430	2.525884
	H	-2.205420	-1.377545	3.241004
	C	-1.944535	-0.206385	1.469669
	H	-3.033205	-0.135305	1.524466
	H	-1.526921	0.799773	1.558267
	C	-1.939181	0.379768	-0.948624
	H	-1.189005	1.163666	-0.789409
	H	-1.782393	-0.086280	-1.925677
	C	-3.328547	0.957678	-0.870117
	C	-4.361224	0.417113	-1.643926

	C	-3.590512	2.073797	-0.068228
	C	-5.642581	0.962821	-1.594208
	H	-4.157272	-0.428526	-2.301793
	C	-4.870488	2.621445	-0.017200
	H	-2.788837	2.524860	0.516519
	C	-5.899557	2.062365	-0.775740
	H	-6.438207	0.536179	-2.202579
	H	-5.064504	3.491804	0.607399
	H	-6.899049	2.493220	-0.740326
	C	0.512826	-1.063232	-1.336338
	H	0.329253	-0.119614	-1.864306
	O	-0.056016	-2.134699	-2.064084
	H	0.381854	-2.192506	-2.923316
	C	2.012718	-1.192914	-1.144890
	C	2.780502	-0.059169	-0.727362
	C	2.657676	-2.387146	-1.336873
	C	2.233528	1.231097	-0.523887
	C	4.173616	-0.263020	-0.512952
	C	4.057386	-2.473104	-1.106572
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	H	5.055815	2.891502	0.450118
	O	2.418833	3.471014	0.072027
	C	3.221900	4.580943	0.457168
	H	2.541706	5.433730	0.513101
	H	3.680438	4.414522	1.441177
	H	3.999561	4.782612	-0.291428
	N	-1.629188	-0.695414	0.073495
	C	-0.205033	-0.704903	3.321477
	H	0.132270	-1.428830	4.067997
	C	0.462309	0.444339	3.220764
	H	1.312880	0.644045	3.870023
	H	0.204722	1.235511	2.516145
	N	4.790472	-1.465538	-0.704117

Compound	Coordinates			
	Atom	x	y	z
conf_3	C	-1.352749	-0.559902	-0.113693
Img. freq. = 0	C	-3.127992	-1.346665	1.467363
SCF Energy (a.u.) = -1307.24148508	C	-1.918854	-1.777353	0.636731

H	-0.600478	-0.068808	0.506947
H	-2.209242	-2.556594	-0.078329
H	-1.121602	-2.179258	1.268893
C	-3.774350	-0.172746	-0.629825
H	-4.468120	0.641441	-0.854212
H	-3.569959	-0.731982	-1.542682
C	-4.286820	-1.064946	0.509935
H	-5.110519	-0.575437	1.042501
H	-4.667988	-1.999010	0.085132
H	-3.398202	-2.124488	2.188104
C	-2.791148	-0.035362	2.204535
H	-3.656679	0.221766	2.829292
C	-2.641650	1.071107	1.145412
H	-3.530657	1.707123	1.087782
H	-1.770825	1.690737	1.343903
C	-2.209393	1.587748	-1.254112
H	-2.256139	1.097285	-2.231929
H	-3.079075	2.246525	-1.155989
C	-0.935160	2.395950	-1.141565
C	-0.733640	3.345639	-0.130008
C	0.016025	2.305648	-2.165580
C	0.431300	4.109467	-0.094804
H	-1.497917	3.525777	0.623410
C	1.176344	3.076154	-2.140337
H	-0.160169	1.633632	-3.005526
C	1.396833	3.964900	-1.090254
H	0.574790	4.834323	0.704515
H	1.905142	2.983118	-2.943323
H	2.308247	4.559241	-1.059696
C	-0.659675	-0.940834	-1.425732
H	-0.205636	-0.049429	-1.866673
O	-1.626932	-1.477315	-2.309516
H	-1.182234	-1.762595	-3.118210
C	0.460791	-1.913676	-1.098138
C	1.650669	-1.456445	-0.442515
C	0.345403	-3.249071	-1.386596
C	1.905658	-0.101606	-0.116639
C	2.620388	-2.444141	-0.101692
C	1.388985	-4.141944	-1.022624
H	-0.542851	-3.643521	-1.875629
C	3.061248	0.255732	0.552548
H	1.221155	0.699014	-0.392316
C	3.798587	-2.043761	0.575654
H	1.293035	-5.203290	-1.256637
C	4.021646	-0.729516	0.906462

	H	4.524391	-2.815239	0.826705
	H	4.934638	-0.456338	1.428069
	O	3.206944	1.572543	0.836350
	C	4.383005	1.982253	1.521639
	H	4.295419	3.065046	1.639136
	H	4.448104	1.512180	2.512267
	H	5.283145	1.750797	0.936791
	N	-2.463602	0.486024	-0.236831
	C	-1.609339	-0.215715	3.127905
	H	-1.775063	-0.977569	3.894304
	C	-0.431130	0.408699	3.112857
	H	0.329453	0.155560	3.849369
	H	-0.155575	1.184096	2.395857
	N	2.476661	-3.769396	-0.397176

Compound	Coordinates			
	Atom	x	y	z
conf_4	C	-1.183964	-0.494349	-0.262896
Img. freq. = 0	C	-3.296584	-1.334055	0.849730
SCF Energy (a.u.) = -1307.24018226	C	-1.810849	-1.601976	0.613571
	H	-0.516322	0.125079	0.341129
	H	-1.710154	-2.565474	0.104798
	H	-1.254218	-1.668273	1.553445
	C	-3.478911	-0.179129	-1.346134
	H	-4.226751	0.617116	-1.419483
	H	-3.172541	-0.473809	-2.348281
	C	-3.985124	-1.362731	-0.513958
	H	-5.072081	-1.290844	-0.404687
	H	-3.753520	-2.302440	-1.025877
	H	-3.713671	-2.102353	1.507742
	C	-3.515040	0.055218	1.476957
	H	-4.591050	0.270050	1.456263
	C	-2.782557	1.101403	0.603070
	H	-3.439025	1.929927	0.321626
	H	-1.905620	1.498552	1.117936
	C	-1.816188	1.562352	-1.647025
	H	-1.631260	1.051892	-2.596567
	H	-2.691450	2.208886	-1.775623
	C	-0.605546	2.380868	-1.267817
	C	-0.620144	3.309095	-0.217501
	C	0.532731	2.304826	-2.079369
	C	0.505534	4.083600	0.055280
	H	-1.516630	3.460573	0.379566
	C	1.653673	3.090503	-1.818183
	H	0.538752	1.629452	-2.935546

	C	1.647879	3.968235	-0.736678
	H	0.482570	4.793571	0.880141
	H	2.530727	3.012955	-2.457762
	H	2.526066	4.573364	-0.518694
	C	-0.344661	-1.041916	-1.425325
	H	0.164576	-0.210206	-1.929149
	O	-1.227274	-1.687546	-2.324558
	H	-0.709019	-2.083165	-3.037447
	C	0.721985	-1.982314	-0.880750
	C	1.863181	-1.485191	-0.170034
	C	0.607486	-3.338563	-1.056015
	C	2.112976	-0.112364	0.069636
	C	2.794464	-2.450850	0.315821
	C	1.602701	-4.208740	-0.537371
	H	-0.244569	-3.768030	-1.579284
	C	3.233197	0.288377	0.774394
	H	1.447993	0.667042	-0.296371
	C	3.933747	-2.007419	1.031580
	H	1.503120	-5.285199	-0.684378
	C	4.157388	-0.672806	1.264146
	H	4.629668	-2.762976	1.391996
	H	5.041202	-0.366040	1.816613
	O	3.381275	1.622082	0.958591
	C	4.524793	2.075362	1.670854
	H	4.439905	3.164222	1.705656
	H	4.535944	1.679729	2.695332
	H	5.451158	1.797743	1.150229
	N	-2.282463	0.485044	-0.684141
	C	-3.045618	0.139784	2.902513
	H	-1.981776	-0.044432	3.079312
	C	-3.842320	0.421662	3.932161
	H	-3.459753	0.463859	4.950711
	H	-4.906152	0.617550	3.789727
	N	2.651963	-3.794745	0.125673

Compound	Coordinates			
	Atom	x	y	z
conf_5	C	0.634771	-0.823780	0.219628
Img. freq. = 0	C	1.659683	-3.059698	0.713761
SCF Energy (a.u.) = -1307.23777803	C	0.674322	-2.002242	1.207458
	H	-0.158476	-0.978186	-0.519602
	H	0.983994	-1.644661	2.196247
	H	-0.338858	-2.403262	1.303406
	C	3.140228	-1.101375	0.226319
	H	3.992466	-1.012354	-0.453615

H	3.173033	-0.300539	0.962917
C	3.072263	-2.496828	0.872502
H	3.800784	-3.168850	0.405114
H	3.327480	-2.409386	1.933367
H	1.544979	-3.986970	1.282428
C	1.422777	-3.340655	-0.781507
H	2.134301	-4.112699	-1.097237
C	1.762180	-2.045586	-1.554947
H	2.715542	-2.132042	-2.083761
H	0.981338	-1.781276	-2.274890
C	2.092629	0.352503	-1.536265
H	2.819004	0.016852	-2.283924
H	1.125880	0.478176	-2.036421
C	2.550602	1.671175	-0.948962
C	1.694868	2.776754	-1.016371
C	3.846157	1.858330	-0.453225
C	2.094459	4.024206	-0.541003
H	0.701942	2.664146	-1.454336
C	4.246901	3.101665	0.031512
H	4.560931	1.039151	-0.449472
C	3.369210	4.185076	0.000225
H	1.412071	4.870275	-0.600953
H	5.254941	3.227333	0.422806
H	3.686000	5.156310	0.376837
C	0.338397	0.510530	0.913170
H	0.287043	1.304965	0.165003
O	1.382301	0.775505	1.827337
H	1.351697	1.709606	2.071141
C	-1.023848	0.420805	1.581736
C	-2.223394	0.520241	0.805827
C	-1.136255	0.235860	2.935532
C	-2.245066	0.754020	-0.590595
C	-3.459966	0.384171	1.501024
C	-2.423086	0.124190	3.526492
H	-0.249545	0.170583	3.562478
C	-3.441646	0.835120	-1.277060
H	-1.330505	0.896866	-1.162760
C	-4.670902	0.466779	0.768923
H	-2.507128	-0.027114	4.603693
C	-4.674357	0.682443	-0.587466
H	-5.603657	0.356603	1.319507
H	-5.619450	0.741201	-1.120029
O	-3.355914	1.065940	-2.608965
C	-4.567563	1.195835	-3.344135
H	-4.268006	1.401641	-4.374365

	H	-5.150848	0.265813	-3.312074
	H	-5.170009	2.031966	-2.965381
	N	1.913952	-0.854005	-0.624247
	C	0.033182	-3.838562	-1.075246
	H	-0.794033	-3.140366	-0.917473
	C	-0.231736	-5.071263	-1.504609
	H	-1.252639	-5.399303	-1.692539
	H	0.565837	-5.794827	-1.679710
	N	-3.541961	0.184077	2.848578

Compound	Coordinates			
	Atom	x	y	z
conf_6	C	-0.377431	0.435635	-0.108370
Img. freq. = 0	C	-0.597756	0.661567	2.374216
SCF Energy (a.u.) = -1307.23753682	C	0.393452	0.534541	1.215346
	H	-0.542755	1.435427	-0.525100
	H	1.004090	-0.361718	1.362333
	H	1.073974	1.389527	1.155630
	C	-1.773547	-1.199953	1.196041
	H	-2.798990	-1.569885	1.255483
	H	-1.135028	-1.969744	0.761489
	C	-1.267073	-0.702166	2.560564
	H	-2.096946	-0.625312	3.271904
	H	-0.548638	-1.426196	2.958560
	H	-0.081436	0.971106	3.287353
	C	-1.693985	1.685643	2.024621
	H	-2.370057	1.767227	2.883971
	C	-2.514525	1.106362	0.845894
	H	-3.481973	0.725571	1.179041
	H	-2.681153	1.846458	0.056893
	C	-2.500438	-0.475577	-1.073557
	H	-2.330940	0.341499	-1.782383
	H	-1.977675	-1.372689	-1.416628
	C	-3.976116	-0.749746	-0.938011
	C	-4.432182	-2.047906	-0.686874
	C	-4.908796	0.276200	-1.128430
	C	-5.797776	-2.311088	-0.592731
	H	-3.714486	-2.861345	-0.575451
	C	-6.273929	0.015762	-1.034470
	H	-4.565401	1.285866	-1.356732
	C	-6.719384	-1.278047	-0.760716
	H	-6.142645	-3.325448	-0.399438
	H	-6.991930	0.820193	-1.185157
	H	-7.786664	-1.483567	-0.692920
	C	0.358761	-0.342753	-1.210633

	H	-0.223966	-0.264681	-2.137722
	O	0.456709	-1.701979	-0.834608
	H	0.999664	-2.167391	-1.484611
	C	1.680188	0.364619	-1.506870
	C	2.955441	0.039551	-0.934584
	C	1.616617	1.411697	-2.395655
	C	3.198668	-1.009419	-0.011157
	C	4.061564	0.850747	-1.345941
	C	2.775815	2.158389	-2.717308
	H	0.672849	1.671579	-2.875869
	C	4.468523	-1.245405	0.478386
	H	2.399674	-1.653929	0.337503
	C	5.351826	0.577909	-0.825146
	H	2.708344	2.990363	-3.419604
	C	5.565442	-0.443363	0.065043
	H	6.171482	1.211198	-1.159756
	H	6.566983	-0.626920	0.443540
	O	4.588350	-2.268751	1.357862
	C	5.880533	-2.547834	1.882338
	H	5.749000	-3.393996	2.560656
	H	6.579262	-2.826930	1.082464
	H	6.273121	-1.688424	2.442525
	N	-1.797161	-0.058275	0.203110
	C	-1.149737	3.058359	1.732867
	H	-0.482688	3.165278	0.873029
	C	-1.428863	4.132696	2.469337
	H	-1.005074	5.107501	2.233924
	H	-2.088103	4.071366	3.336434
	N	3.956572	1.893324	-2.217767

Compound	Coordinates			
	Atom	x	y	z
conf_7	C	-0.538712	0.842968	0.295033
Img. freq. = 0	C	-1.124386	3.178488	0.948971
SCF Energy (a.u.) = -1307.23823961	C	-0.424325	1.898415	1.404276
	H	0.293834	0.963488	-0.402091
	H	-0.877814	1.522854	2.329661
	H	0.639646	2.066778	1.595838
	C	-2.938128	1.590080	0.304700
	H	-3.792845	1.671623	-0.370677
	H	-3.106086	0.779637	1.012868
	C	-2.633068	2.931099	0.994193
	H	-3.168463	3.748760	0.497755
	H	-2.981396	2.881602	2.030689
	H	-0.848890	4.021749	1.589192

C	-0.730232	3.474492	-0.513886
H	-1.195260	4.430029	-0.789763
C	-1.374631	2.386629	-1.388940
H	-2.302938	2.742600	-1.846275
H	-0.715277	2.026177	-2.182310
C	-2.159848	0.099659	-1.560803
H	-2.796709	0.622103	-2.282934
H	-1.228425	-0.173039	-2.067977
C	-2.871702	-1.148102	-1.081822
C	-2.233625	-2.387368	-1.211615
C	-4.197976	-1.123919	-0.634557
C	-2.874870	-3.567340	-0.838505
H	-1.223862	-2.438151	-1.620302
C	-4.839717	-2.300238	-0.252340
H	-4.753870	-0.189814	-0.595063
C	-4.176260	-3.523632	-0.340047
H	-2.360824	-4.520543	-0.948770
H	-5.868453	-2.261875	0.101364
H	-4.681175	-4.442077	-0.044887
C	-0.470562	-0.588862	0.829800
H	-0.498150	-1.286663	-0.010497
O	-1.570220	-0.809843	1.687958
H	-1.791211	-1.749849	1.677709
C	0.866636	-0.765420	1.531979
C	2.084858	-0.831593	0.781083
C	0.938884	-0.825517	2.899063
C	2.147668	-0.825642	-0.633849
C	3.300057	-0.906439	1.521644
C	2.205824	-0.928552	3.533374
H	0.034566	-0.786170	3.502085
C	3.362289	-0.853336	-1.291125
H	1.251909	-0.823365	-1.251207
C	4.530980	-0.937910	0.819463
H	2.257701	-0.978150	4.622091
C	4.574848	-0.903399	-0.553037
H	5.446479	-0.990739	1.406330
H	5.534813	-0.927798	-1.060562
O	3.312518	-0.832461	-2.645697
C	4.545023	-0.872519	-3.355692
H	4.278622	-0.854725	-4.415002
H	5.164194	0.003407	-3.120233
H	5.097277	-1.795039	-3.133692
N	-1.768859	1.174552	-0.558365
C	0.762886	3.650585	-0.655329
H	1.164537	4.438570	-0.012745

	C	1.613947	2.983970	-1.434996
	H	2.675017	3.226524	-1.422600
	H	1.317076	2.186201	-2.116651
	N	3.343494	-0.953873	2.885271

Compound	Coordinates			
	Atom	x	y	z
conf_8	C	0.748199	0.322316	-0.161740
Img. freq. = 0	C	0.428882	2.791207	0.311785
SCF Energy (a.u.) = -1307.23586254	C	-0.060126	1.376664	0.631411
	H	1.256554	-0.361553	0.524135
	H	-1.115458	1.304328	0.359588
	H	0.010865	1.159143	1.701507
	C	1.432859	2.091747	-1.852178
	H	2.339372	2.654739	-2.098347
	H	1.072882	1.583815	-2.746327
	C	0.362456	2.979011	-1.205354
	H	0.552844	4.022736	-1.475766
	H	-0.629140	2.701450	-1.575514
	H	-0.200367	3.526917	0.820972
	C	1.897747	2.965611	0.738680
	H	2.286055	3.871329	0.255366
	C	2.680445	1.745684	0.209787
	H	3.636131	2.042962	-0.229576
	H	2.865629	1.013194	0.999964
	C	2.810902	0.086487	-1.641054
	H	2.216932	-0.295978	-2.475892
	H	3.594382	0.733850	-2.049871
	C	3.411951	-1.051166	-0.851340
	C	4.482979	-0.839098	0.026830
	C	2.960772	-2.360258	-1.054257
	C	5.046232	-1.901332	0.729741
	H	4.898456	0.158872	0.154555
	C	3.527116	-3.426860	-0.356545
	H	2.176216	-2.562471	-1.782303
	C	4.561652	-3.196980	0.548242
	H	5.875750	-1.718349	1.410685
	H	3.165665	-4.439276	-0.529159
	H	5.005611	-4.027249	1.095056
	C	-0.103938	-0.574819	-1.071038
	H	0.556557	-1.314165	-1.537688
	O	-0.705499	0.208392	-2.082194
	H	-1.301162	-0.353202	-2.595372
	C	-1.064090	-1.382317	-0.195309
	C	-2.446149	-1.078025	0.047142

	C	-0.529887	-2.494052	0.414495
	C	-3.153619	0.031645	-0.486377
	C	-3.153732	-1.978725	0.907116
	C	-1.322868	-3.306317	1.259312
	H	0.513135	-2.767631	0.250384
	C	-4.487121	0.235604	-0.190849
	H	-2.668558	0.756079	-1.131305
	C	-4.523381	-1.738969	1.187160
	H	-0.882096	-4.181686	1.738691
	C	-5.187833	-0.662833	0.657747
	H	-5.029578	-2.443647	1.844554
	H	-6.236760	-0.506303	0.893629
	O	-5.061122	1.327795	-0.750519
	C	-6.436177	1.570550	-0.480687
	H	-6.689146	2.481798	-1.027511
	H	-7.061926	0.743384	-0.842135
	H	-6.606233	1.730312	0.592636
	N	1.901012	1.029781	-0.874531
	C	2.094106	3.109867	2.221308
	H	1.750970	2.282680	2.849207
	C	2.656324	4.173454	2.793873
	H	2.771554	4.240501	3.874452
	H	3.015937	5.015244	2.200395
	N	-2.588199	-3.068338	1.498143

Compound	Coordinates			
	Atom	x	y	z
conf_9	C	-0.381189	0.444813	0.148345
Img. freq. = 0	C	-0.580253	-0.366117	2.504397
SCF Energy (a.u.) = -1307.23778598	C	0.401901	-0.021458	1.382950
	H	-0.532047	1.529809	0.192427
	H	1.001182	-0.904687	1.141477
	H	1.087524	0.780855	1.671868
	C	-1.776988	-1.572644	0.679619
	H	-2.798351	-1.943746	0.579341
	H	-1.128973	-2.088782	-0.029147
	C	-1.276614	-1.675923	2.130321
	H	-2.111819	-1.871999	2.812532
	H	-0.576773	-2.514258	2.205415
	H	-0.054138	-0.463374	3.458812
	C	-1.653502	0.736356	2.604164
	H	-2.307821	0.478142	3.447403
	C	-2.510448	0.668428	1.326347
	H	-3.455630	0.152142	1.509282
	H	-2.732529	1.651883	0.905552

C	-2.530043	0.029051	-1.077462
H	-2.385931	1.074490	-1.372873
H	-2.005989	-0.628016	-1.776381
C	-4.000031	-0.303000	-1.049489
C	-4.439583	-1.591438	-1.371340
C	-4.945755	0.688403	-0.766491
C	-5.800457	-1.893111	-1.376529
H	-3.713601	-2.362767	-1.630053
C	-6.306371	0.389857	-0.771104
H	-4.616275	1.704534	-0.548657
C	-6.734645	-0.904015	-1.070093
H	-6.131708	-2.898833	-1.629886
H	-7.033596	1.169520	-0.551097
H	-7.798323	-1.137247	-1.078463
C	0.329164	0.183434	-1.188703
H	-0.265050	0.644785	-1.988492
O	0.407265	-1.211849	-1.410542
H	0.940067	-1.372636	-2.200566
C	1.659514	0.934616	-1.195339
C	2.932554	0.392104	-0.814822
C	1.609029	2.250500	-1.590861
C	3.164167	-0.943022	-0.396022
C	4.048529	1.287121	-0.872318
C	2.778634	3.048437	-1.598601
H	0.666723	2.694236	-1.914192
C	4.430761	-1.370144	-0.048550
H	2.358447	-1.666084	-0.339822
C	5.335256	0.814031	-0.510360
H	2.720915	4.092044	-1.910879
C	5.536898	-0.481077	-0.106023
H	6.162108	1.519722	-0.566861
H	6.536502	-0.812227	0.161726
O	4.537010	-2.663395	0.340895
C	5.826112	-3.151127	0.691334
H	5.683194	-4.200538	0.959444
H	6.518599	-3.082989	-0.158509
H	6.234940	-2.607909	1.554255
N	-1.806187	-0.122970	0.246765
C	-1.029375	2.072865	2.922185
H	-0.439726	2.064801	3.842723
C	-1.110853	3.214126	2.239586
H	-0.601817	4.107872	2.595715
H	-1.685000	3.321422	1.319131
N	3.956505	2.592313	-1.254608

Compound	Coordinates			
	Atom	x	y	z
conf_10	C	-0.716071	-0.410975	-0.174208
Img. freq. = 0	C	-0.353019	-2.833071	0.458439
SCF Energy (a.u.) = -1307.23551335	C	0.109035	-1.394828	0.689123
	H	-1.233930	0.311782	0.463908
	H	1.165763	-1.312982	0.427584
	H	0.006963	-1.125235	1.744977
	C	-1.366285	-2.288456	-1.749214
	H	-2.262054	-2.868909	-1.993212
	H	-0.988283	-1.818546	-2.656542
	C	-0.300387	-3.133699	-1.039931
	H	-0.499369	-4.194000	-1.227344
	H	0.690290	-2.892750	-1.435871
	H	0.293499	-3.522158	1.010773
	C	-1.810939	-2.977745	0.932638
	H	-2.183797	-3.938907	0.552595
	C	-2.628894	-1.847240	0.290662
	H	-3.556515	-2.222918	-0.148490
	H	-2.866902	-1.053094	0.997838
	C	-2.798692	-0.312248	-1.649286
	H	-2.205285	0.087934	-2.475819
	H	-3.528438	-1.015891	-2.062868
	C	-3.498189	0.798563	-0.903082
	C	-4.636041	0.541350	-0.125899
	C	-3.071286	2.122895	-1.046403
	C	-5.292286	1.575268	0.537211
	H	-5.030442	-0.470503	-0.047992
	C	-3.728120	3.161243	-0.386381
	H	-2.234345	2.359567	-1.702162
	C	-4.832130	2.887194	0.418268
	H	-6.174782	1.357844	1.136409
	H	-3.382528	4.186266	-0.511142
	H	-5.347787	3.695680	0.933924
	C	0.132924	0.423510	-1.147770
	H	-0.531893	1.100187	-1.698385
	O	0.779281	-0.433738	-2.067492
	H	1.376360	0.094015	-2.613860
	C	1.059517	1.333473	-0.337902
	C	2.444615	1.088653	-0.047036
	C	0.493440	2.490783	0.143754
	C	3.188840	-0.049188	-0.457436
	C	3.118074	2.091125	0.723640
	C	1.252426	3.402641	0.914563
	H	-0.550279	2.723510	-0.067238

	C	4.524551	-0.182766	-0.133104
	H	2.733562	-0.849008	-1.030748
	C	4.490840	1.920965	1.037008
	H	0.784007	4.311061	1.295950
	C	5.191393	0.817572	0.623009
	H	4.970222	2.703570	1.622323
	H	6.242466	0.718596	0.879305
	O	5.134841	-1.309664	-0.572653
	C	6.522552	-1.464767	-0.302946
	H	6.808025	-2.415703	-0.758568
	H	7.105846	-0.653088	-0.758419
	H	6.714360	-1.505885	0.777808
	N	-1.859517	-1.186291	-0.833791
	C	-1.903074	-3.028834	2.435458
	H	-1.405962	-3.900321	2.868882
	C	-2.486143	-2.161621	3.263424
	H	-2.457130	-2.332001	4.338363
	H	-3.016239	-1.267927	2.935164
	N	2.518334	3.220326	1.194422

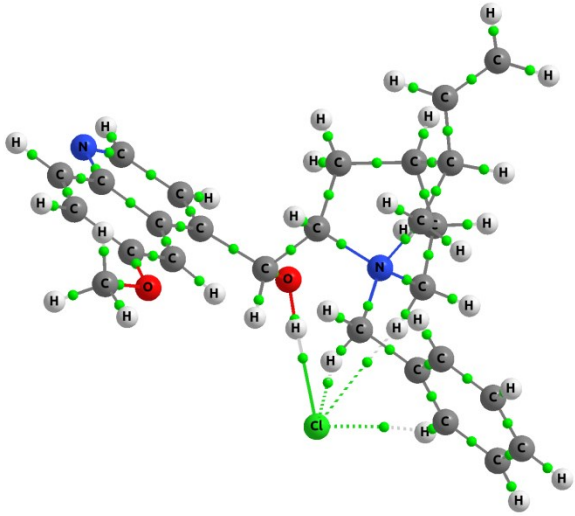
Compound	Coordinates			
	Atom	x	y	z
conf_11	C	0.823130	0.844876	0.354585
Img. freq. = 0	C	0.771325	2.643737	-1.390050
SCF Energy (a.u.) = -1307.23100139	C	-0.075219	1.645776	-0.600811
	H	0.889864	1.351349	1.324370
	H	-0.575830	0.968079	-1.299499
	H	-0.851514	2.139899	-0.008715
	C	2.306296	0.689655	-1.673809
	H	3.367234	0.643185	-1.932007
	H	1.840318	-0.275857	-1.865505
	C	1.600441	1.848756	-2.399958
	H	2.335947	2.501261	-2.883770
	H	0.952957	1.435191	-3.179740
	H	0.132746	3.372251	-1.897371
	C	1.746643	3.374540	-0.449533
	H	2.320167	4.090200	-1.050639
	C	2.740956	2.319270	0.089097
	H	3.712573	2.400237	-0.406593
	H	2.887580	2.402150	1.170936
	C	3.241875	-0.005266	0.556061
	H	4.225475	0.411670	0.313895
	H	3.052428	0.172434	1.620354
	C	3.244644	-1.491823	0.268419
	C	2.909982	-2.384336	1.293308

C	3.692306	-2.013280	-0.950941
C	2.948345	-3.761922	1.086189
H	2.623285	-2.002178	2.273521
C	3.724439	-3.389703	-1.164697
H	4.033701	-1.354018	-1.745227
C	3.338887	-4.268184	-0.152682
H	2.682753	-4.438919	1.896221
H	4.066296	-3.777690	-2.122531
H	3.365782	-5.343466	-0.321730
C	0.298866	-0.562090	0.654989
H	0.969239	-1.013245	1.391015
O	0.315968	-1.322555	-0.532925
H	0.256113	-2.259791	-0.306254
C	-1.055648	-0.449758	1.354971
C	-2.338138	-0.502568	0.713962
C	-1.021033	-0.256621	2.716099
C	-2.551116	-0.717585	-0.671132
C	-3.481000	-0.324567	1.557720
C	-2.218602	-0.088307	3.453429
H	-0.069244	-0.237215	3.248945
C	-3.827638	-0.743303	-1.197207
H	-1.720394	-0.883309	-1.346866
C	-4.776879	-0.357592	0.983647
H	-2.174116	0.070001	4.531911
C	-4.960972	-0.558893	-0.360882
H	-5.624778	-0.217623	1.651631
H	-5.967700	-0.580009	-0.769214
O	-3.918277	-0.954010	-2.533274
C	-5.216181	-1.010574	-3.110314
H	-5.060184	-1.197465	-4.175378
H	-5.804734	-1.830884	-2.677990
H	-5.747755	-0.058227	-2.980871
N	2.261083	0.901803	-0.176957
C	1.057291	4.143302	0.645814
H	0.506853	3.572479	1.399285
C	1.081524	5.472169	0.735496
H	0.559767	5.996595	1.534230
H	1.621955	6.080326	0.008506
N	-3.406149	-0.115966	2.903248

Compound	Coordinates			
	Atom	x	y	z
conf_12	C	0.813715	0.929502	0.184044
Img. freq. = 0	C	0.730372	2.543258	-1.725684
SCF Energy (a.u.) = -1307.23118858	C	-0.098276	1.599699	-0.854214

H	0.861112	1.544951	1.088453
H	-0.572198	0.840532	-1.485117
H	-0.889108	2.129993	-0.315046
C	2.307182	0.610429	-1.813894
H	3.370614	0.553684	-2.057461
H	1.850897	-0.373886	-1.912895
C	1.595487	1.687120	-2.650630
H	2.328761	2.312570	-3.172738
H	0.974114	1.195134	-3.405593
H	0.079349	3.204200	-2.305402
C	1.666293	3.377242	-0.829634
H	2.211780	4.070255	-1.484102
C	2.699899	2.414058	-0.222741
H	3.654858	2.467395	-0.753230
H	2.882058	2.598886	0.838793
C	3.252183	0.156330	0.464946
H	4.226308	0.567351	0.176102
H	3.061032	0.433902	1.507445
C	3.279751	-1.352273	0.332027
C	3.001726	-2.125122	1.465538
C	3.691197	-2.004937	-0.837279
C	3.065861	-3.516347	1.421752
H	2.736434	-1.634186	2.402489
C	3.749416	-3.396534	-0.885931
H	3.982036	-1.444820	-1.722183
C	3.425528	-4.157083	0.237306
H	2.842892	-4.097206	2.315100
H	4.062822	-3.889780	-1.804342
H	3.473461	-5.244037	0.195561
C	0.318055	-0.446930	0.632451
H	1.002186	-0.817160	1.401087
O	0.331773	-1.322050	-0.473798
H	0.283566	-2.232430	-0.154258
C	-1.027374	-0.265411	1.336550
C	-2.320511	-0.412973	0.733440
C	-0.969869	0.113071	2.657459
C	-2.555924	-0.808208	-0.607804
C	-3.449553	-0.133548	1.568181
C	-2.155355	0.370544	3.388065
H	-0.009597	0.215341	3.164546
C	-3.841229	-0.916510	-1.100518
H	-1.734288	-1.049179	-1.271750
C	-4.755114	-0.255560	1.029055
H	-2.092435	0.676389	4.433389
C	-4.961050	-0.636427	-0.272754

	H	-5.592658	-0.035671	1.688578
	H	-5.974484	-0.723032	-0.654975
	O	-3.953950	-1.300482	-2.396029
	C	-5.261127	-1.459307	-2.931351
	H	-5.121669	-1.786778	-3.964339
	H	-5.823335	-2.224854	-2.379521
	H	-5.812127	-0.508959	-2.921210
	N	2.251888	0.966621	-0.346719
	C	0.881371	4.216227	0.148363
	H	0.159591	4.879225	-0.336087
	C	0.963866	4.244368	1.478039
	H	0.325565	4.912326	2.053557
	H	1.656682	3.630763	2.053931
	N	-3.352732	0.256418	2.871167

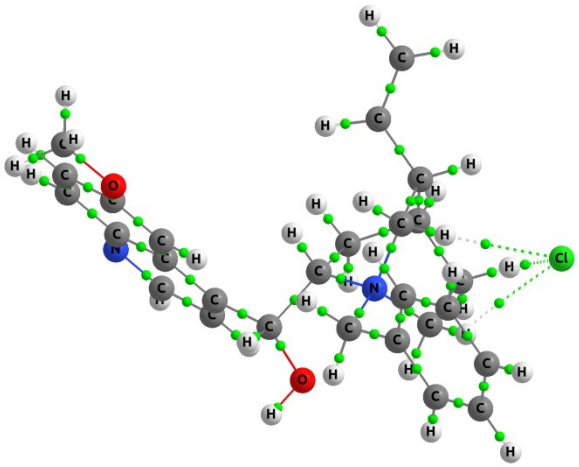
Compound	Coordinates			
	Atom	x	y	z
complex_Cl_1	C	0.074137	-0.957664	0.114023
Img. freq. = 0	C	-1.231866	-2.994015	0.842998
SCF Energy (a.u.) = -1767.65031289	C	0.165236	-2.419295	0.607539
	H	0.547888	-0.282346	0.832801
	H	0.667385	-3.019709	-0.156712
	H	0.774894	-2.463431	1.515679
	C	-2.278583	-1.364028	-0.735397
	H	-3.299459	-1.070856	-0.475971
	H	-2.080368	-1.074155	-1.769965
	C	-2.025392	-2.852972	-0.458371
	H	-2.986377	-3.372842	-0.379879
	H	-1.458444	-3.287945	-1.286307
	H	-1.160419	-4.045301	1.139865
	C	-1.957598	-2.191565	1.937921
	H	-3.016306	-2.481184	1.929423
	C	-1.851703	-0.695170	1.571600
	H	-2.819625	-0.201358	1.665338
	H	-1.123773	-0.169471	2.199346
	C	-1.485477	0.950223	-0.248393
	H	-0.782224	1.473098	0.408790
	H	-1.155573	1.002517	-1.289545
	C	-2.863205	1.554587	-0.144003
	C	-3.725934	1.504000	-1.244906
	C	-3.268318	2.226728	1.014600
	C	-4.989885	2.087740	-1.170752
	H	-3.388713	1.024503	-2.165587
	C	-4.530414	2.813041	1.087558
	H	-2.586795	2.301111	1.863064

C	-5.395885	2.736932	-0.004442
H	-5.653522	2.047551	-2.033143
H	-4.835108	3.337656	1.991942
H	-6.381271	3.198246	0.048571
C	0.776962	-0.768688	-1.252474
H	0.605886	0.243553	-1.639481
O	0.318194	-1.707001	-2.185370
H	-0.171413	-1.197685	-2.877338
C	2.269983	-0.929539	-1.007780
C	3.027803	0.079449	-0.329440
C	2.925812	-2.064041	-1.410237
C	2.487635	1.323090	0.078212
C	4.403376	-0.191285	-0.075791
C	4.305528	-2.225941	-1.116255
H	2.392581	-2.836699	-1.958852
C	3.269496	2.253015	0.734273
H	1.457247	1.591551	-0.143877
C	5.178991	0.781094	0.602718
H	4.817345	-3.135719	-1.435183
C	4.635323	1.976542	1.007610
H	6.227411	0.552617	0.787654
H	5.258282	2.703533	1.521144
O	2.659870	3.414542	1.085862
C	3.449559	4.414325	1.712231
H	2.778709	5.259894	1.882979
H	3.844809	4.062943	2.675442
H	4.275772	4.731327	1.061451
N	-1.393130	-0.514034	0.147845
C	-1.418484	-2.433431	3.318630
H	-0.366669	-2.184351	3.486134
C	-2.140553	-2.921888	4.326537
H	-1.703268	-3.087263	5.310161
H	-3.194340	-3.174113	4.199314
N	5.023613	-1.344370	-0.465056
Cl	-1.268336	0.279728	-3.790586

Compound	Coordinates			
	Atom	x	y	z
complex_Cl_2	C	-0.190133	-0.899643	0.109872
Img. freq. = 0	C	-1.079867	-2.244228	2.023963
SCF Energy (a.u.) = -1767.63806209	C	0.102539	-2.059136	1.072271
	H	0.156495	0.056137	0.521296
	H	0.267673	-2.986064	0.509075
	H	1.026653	-1.832249	1.613050
	C	-2.428764	-2.040667	-0.064990

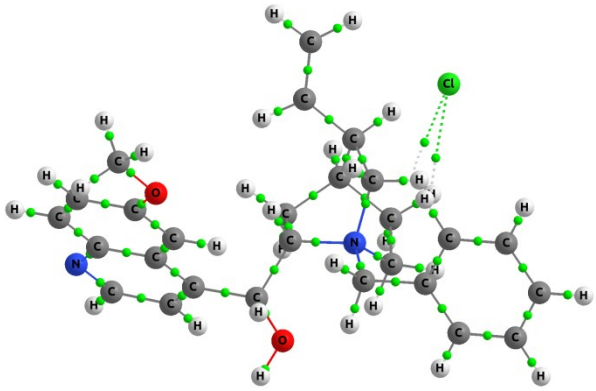
H	-3.480973	-1.799506	-0.227731
H	-2.029937	-2.541208	-0.946225
C	-2.230420	-2.858030	1.223765
H	-3.149285	-2.860142	1.821747
H	-1.999998	-3.895653	0.958582
H	-0.800041	-2.887013	2.864586
C	-1.549623	-0.874860	2.550800
H	-2.366415	-1.055209	3.260877
C	-2.127696	-0.082704	1.355419
H	-3.220012	-0.095435	1.360459
H	-1.765559	0.950590	1.328152
C	-2.078552	0.188027	-1.125515
H	-1.406413	1.048755	-1.037405
H	-1.859936	-0.394542	-2.023663
C	-3.510237	0.658914	-1.133248
C	-4.500546	-0.054756	-1.817342
C	-3.845857	1.862670	-0.501771
C	-5.815946	0.407216	-1.843156
H	-4.239201	-0.971888	-2.346799
C	-5.160922	2.324024	-0.526762
H	-3.061593	2.438128	-0.006134
C	-6.148477	1.594693	-1.190722
H	-6.579296	-0.153462	-2.380882
H	-5.412597	3.262591	-0.035124
H	-7.174690	1.959563	-1.213050
C	0.503077	-1.042542	-1.258631
H	0.434517	-0.083015	-1.789310
O	-0.162345	-2.055735	-2.001379
H	0.303618	-2.167658	-2.839744
C	1.975745	-1.385621	-1.064180
C	2.959047	-0.391618	-0.745121
C	2.393594	-2.686410	-1.208739
C	2.669146	0.984341	-0.585720
C	4.307967	-0.843006	-0.599161
C	3.760604	-3.021537	-1.033642
H	1.685438	-3.475463	-1.451333
C	3.686773	1.882763	-0.309472
H	1.656632	1.385850	-0.651225
C	5.318638	0.100950	-0.298688
H	4.077400	-4.059960	-1.145825
C	5.026646	1.434889	-0.156851
H	6.337654	-0.266661	-0.189782
H	5.825060	2.137214	0.066249
O	3.333798	3.182651	-0.206996
C	4.331672	4.123955	0.148104

H	3.818482	5.086319	0.213559
H	4.776862	3.882593	1.123520
H	5.117892	4.181332	-0.618176
N	-1.713979	-0.716867	0.041087
C	-0.465432	-0.117556	3.272169
H	0.297913	0.374531	2.663840
C	-0.409741	-0.008386	4.598877
H	0.391801	0.542039	5.088587
H	-1.171616	-0.457761	5.238589
N	4.688576	-2.146765	-0.739455
Cl	-0.329984	2.705700	0.439802

Compound	Coordinates			
	Atom	x	y	z
complex_Cl_3	C	0.200528	-0.798949	-0.212006
Img. freq. = 0	C	-0.968026	-2.499855	1.201284
SCF Energy (a.u.) = -1767.63155006	C	0.312360	-2.194069	0.422732
	H	0.638910	-0.052072	0.458334
	H	0.451286	-2.947146	-0.362041
	H	1.200185	-2.214010	1.062389
	C	-2.158138	-1.525188	-0.768644
	H	-3.173330	-1.120277	-0.774930
	H	-1.816427	-1.753689	-1.778559
	C	-2.086325	-2.728313	0.185408
	H	-3.051578	-2.826823	0.693074
	H	-1.886636	-3.638693	-0.390878
	H	-0.829202	-3.384548	1.830717
	C	-1.355497	-1.298085	2.085556
	H	-2.285102	-1.552178	2.609105
	C	-1.683296	-0.103639	1.160622
	H	-2.764444	0.068833	1.144133
	H	-1.147878	0.805926	1.453829
	C	-1.450104	0.828643	-1.129854
	H	-0.710684	1.552709	-0.767912
	H	-1.194081	0.516386	-2.145849
	C	-2.829894	1.432500	-1.115058
	C	-3.770809	1.049941	-2.075160
	C	-3.175182	2.403202	-0.170785
	C	-5.047865	1.605393	-2.073635
	H	-3.506559	0.302870	-2.823941
	C	-4.451482	2.959985	-0.166487
	H	-2.445736	2.721489	0.573948
	C	-5.391387	2.556413	-1.114113
	H	-5.778889	1.286919	-2.814596
	H	-4.716634	3.702189	0.584363

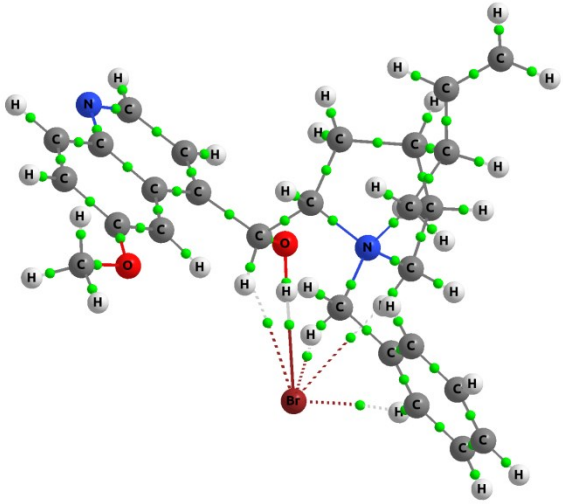
	H	-6.394362	2.980011	-1.101273
	C	0.965572	-0.681643	-1.541103
	H	0.916645	0.351241	-1.910231
	O	0.366524	-1.553269	-2.480660
	H	0.859173	-1.499045	-3.309469
	C	2.427517	-1.009268	-1.285093
	C	3.291780	-0.058259	-0.651966
	C	2.950667	-2.227645	-1.635419
	C	2.882406	1.239781	-0.263957
	C	4.637747	-0.459135	-0.410422
	C	4.313021	-2.518167	-1.356732
	H	2.332232	-2.984667	-2.113164
	C	3.765144	2.104652	0.354041
	H	1.872390	1.598325	-0.447798
	C	5.519510	0.449631	0.225172
	H	4.721133	-3.490546	-1.636947
	C	5.103933	1.702343	0.606385
	H	6.542641	0.121925	0.401517
	H	5.804636	2.375466	1.092252
	O	3.277664	3.323731	0.688955
	C	4.158809	4.242575	1.321378
	H	3.568989	5.144940	1.498715
	H	4.519284	3.847876	2.280933
	H	5.009878	4.484881	0.670681
	N	-1.274037	-0.401239	-0.266111
	C	-0.298927	-0.960597	3.100960
	H	0.663887	-0.599826	2.724555
	C	-0.470579	-1.077052	4.417420
	H	0.325301	-0.830390	5.118762
	H	-1.418181	-1.421908	4.833463
	N	5.129260	-1.682693	-0.764991
	Cl	-4.987989	-0.925501	1.190296

Compound	Coordinates			
	Atom	x	y	z
complex_Cl_5	C	0.180600	-0.933268	0.320260
Img. freq. = 0	C	-0.833122	-1.353996	2.565277
SCF Energy (a.u.) = -1767.62666609	C	0.397623	-1.601079	1.686443
	H	0.530639	0.103151	0.354575
	H	0.554271	-2.678877	1.553038
	H	1.306928	-1.188165	2.132373
	C	-2.058431	-2.049070	0.505156
	H	-3.091094	-1.916603	0.178019
	H	-1.602585	-2.870350	-0.049274
	C	-1.966527	-2.232656	2.029352



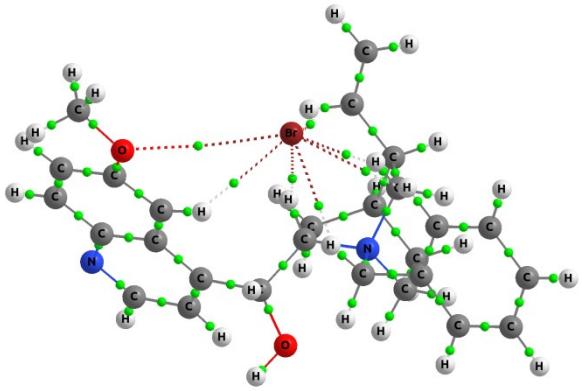
H	-2.914497	-1.955310	2.503550
H	-1.771859	-3.288042	2.249200
H	-0.612761	-1.595696	3.609514
C	-1.275062	0.117394	2.446852
H	-2.137628	0.289570	3.100138
C	-1.784443	0.331981	1.003013
H	-2.873220	0.348312	0.972443
H	-1.422478	1.268066	0.571734
C	-1.617347	-0.451935	-1.349469
H	-1.015354	0.437437	-1.567943
H	-1.253454	-1.298741	-1.936691
C	-3.072339	-0.216165	-1.671878
C	-3.792756	-1.224294	-2.323694
C	-3.707619	0.993160	-1.369768
C	-5.131186	-1.034848	-2.660626
H	-3.299346	-2.165119	-2.571489
C	-5.050175	1.177765	-1.695588
H	-3.183865	1.791561	-0.844829
C	-5.762409	0.168198	-2.342250
H	-5.680790	-1.825143	-3.169956
H	-5.536578	2.114385	-1.428861
H	-6.810709	0.318120	-2.597403
C	0.962361	-1.607056	-0.819054
H	0.835155	-1.030325	-1.744666
O	0.457975	-2.917616	-0.999972
H	0.973250	-3.352657	-1.691297
C	2.439298	-1.589064	-0.464498
C	3.205723	-0.384792	-0.583454
C	3.066758	-2.716621	0.000280
C	2.683164	0.837872	-1.068511
C	4.572801	-0.442198	-0.183050
C	4.440423	-2.663581	0.357144
H	2.522890	-3.652126	0.114345
C	3.477160	1.966819	-1.139174
H	1.653306	0.930864	-1.405712
C	5.361310	0.731973	-0.267352
H	4.933407	-3.564257	0.726462
C	4.836283	1.914562	-0.728068
H	6.401615	0.665914	0.046703
H	5.465663	2.798703	-0.778362
O	2.886448	3.086732	-1.616647
C	3.658757	4.279182	-1.666997
H	2.988472	5.049845	-2.054294
H	4.005157	4.567364	-0.665393
H	4.515736	4.165928	-2.344634

	N	-1.323684	-0.795031	0.094148
	C	-0.201244	1.094907	2.846205
	H	0.766612	1.034839	2.339841
	C	-0.379476	2.034533	3.773180
	H	0.416467	2.731232	4.032721
	H	-1.337423	2.152654	4.279990
	N	5.170076	-1.579013	0.280515
	Cl	-3.700402	2.705441	1.835181

Compound	Coordinates			
	Atom	x	y	z
complex_Br_1	C	-0.171842	1.111632	-0.010356
Img. freq. = 0	C	1.148079	3.265388	-0.087087
SCF Energy (a.u.) = -3881.69196913	C	-0.252866	2.651681	-0.114147
	H	-0.688583	0.761945	0.888083
	H	-0.734937	2.917833	-1.059165
	H	-0.877021	3.043229	0.695537
	C	2.208906	1.139155	-0.862407
	H	3.217999	0.965552	-0.478455
	H	2.031969	0.467451	-1.706452
	C	1.973566	2.618775	-1.202572
	H	2.941190	3.122170	-1.303061
	H	1.438362	2.696106	-2.152805
	H	1.086090	4.348736	-0.231234
	C	1.836861	2.955424	1.253943
	H	2.901903	3.201882	1.155017
	C	1.703033	1.438387	1.507018
	H	2.655516	1.012037	1.824608
	H	0.944076	1.213025	2.264579
	C	1.361539	-0.790206	0.479052
	H	0.630546	-1.003938	1.266424
	H	1.059574	-1.255450	-0.463365
	C	2.722699	-1.310068	0.866482
	C	3.627166	-1.699588	-0.127664
	C	3.070848	-1.472574	2.212023
	C	4.875555	-2.211599	0.223229
	H	3.336554	-1.621349	-1.176812
	C	4.317452	-1.987051	2.562955
	H	2.357479	-1.203905	2.992121
	C	5.224499	-2.350691	1.566804
	H	5.571131	-2.516679	-0.556975
	H	4.577523	-2.113615	3.612838
	H	6.197622	-2.757725	1.838680
	C	-0.824649	0.418161	-1.230752
	H	-0.627658	-0.660387	-1.219207

	O	-0.341725	0.962140	-2.430279
	H	0.117106	0.234676	-2.906706
	C	-2.327339	0.621767	-1.105936
	C	-3.099430	-0.107425	-0.144277
	C	-2.978876	1.531194	-1.898035
	C	-2.562261	-1.120796	0.685840
	C	-4.486506	0.202521	-0.045120
	C	-4.370450	1.753211	-1.722818
	H	-2.434405	2.077103	-2.664783
	C	-3.359596	-1.785231	1.596609
	H	-1.521840	-1.427459	0.604379
	C	-5.277614	-0.493226	0.902237
	H	-4.879013	2.484177	-2.353929
	C	-4.737742	-1.462728	1.712919
	H	-6.334665	-0.239022	0.962573
	H	-5.372747	-1.981089	2.425984
	O	-2.751843	-2.739317	2.347639
	C	-3.560495	-3.503748	3.229535
	H	-2.890186	-4.232817	3.691431
	H	-4.004997	-2.871580	4.010761
	H	-4.351582	-4.033027	2.681029
	N	1.284246	0.711164	0.254502
	C	1.284227	3.733980	2.413164
	H	0.224627	3.588629	2.642440
	C	2.003382	4.571262	3.159916
	H	1.556021	5.121100	3.986667
	H	3.064303	4.736362	2.966143
	N	-5.103279	1.135156	-0.829799
	Br	1.262884	-1.688184	-3.213471

Compound	Coordinates			
	Atom	x	y	z
complex_Br_2	C	-0.180285	-1.147507	0.092537
Img. freq. = 0	C	-1.181572	-2.545250	1.916047
SCF Energy (a.u.) = -3881.68059583	C	0.053567	-2.333198	1.040599
	H	0.169548	-0.206745	0.537982
	H	0.248296	-3.244308	0.462612
	H	0.944834	-2.124923	1.640395
	C	-2.431217	-2.239014	-0.225358
	H	-3.472789	-1.969056	-0.409255
	H	-2.013798	-2.706490	-1.115768
	C	-2.290122	-3.118006	1.030433
	H	-3.236549	-3.149991	1.582771
	H	-2.043398	-4.141276	0.727020
	H	-0.951842	-3.224510	2.743053

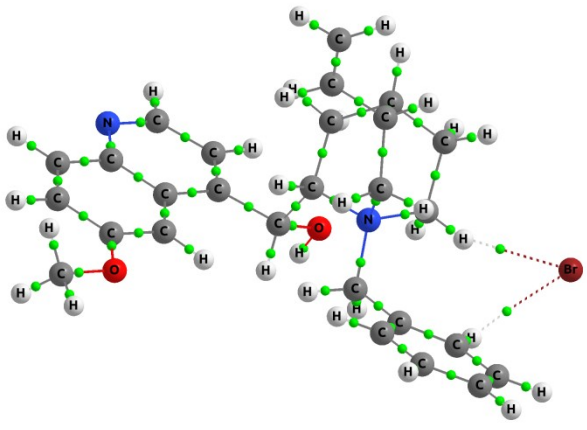


C	-1.669218	-1.195321	2.473919
H	-2.528155	-1.395923	3.126411
C	-2.166373	-0.345482	1.282331
H	-3.257297	-0.334556	1.228874
H	-1.786829	0.681282	1.319845
C	-1.988466	0.022683	-1.177094
H	-1.316291	0.873459	-1.016153
H	-1.721159	-0.521227	-2.086700
C	-3.415034	0.502723	-1.251696
C	-4.360420	-0.177204	-2.027461
C	-3.789281	1.677957	-0.589506
C	-5.671219	0.289486	-2.115643
H	-4.066734	-1.072028	-2.577675
C	-5.099812	2.144589	-0.677601
H	-3.040412	2.229984	-0.018106
C	-6.043579	1.448594	-1.434183
H	-6.399294	-0.244947	-2.724196
H	-5.381198	3.061274	-0.161439
H	-7.066088	1.817575	-1.505256
C	0.561066	-1.282499	-1.252243
H	0.499331	-0.327448	-1.789899
O	-0.067449	-2.304810	-2.014017
H	0.443861	-2.432942	-2.823168
C	2.030976	-1.603148	-1.011941
C	2.999460	-0.580099	-0.747773
C	2.465118	-2.905199	-1.075866
C	2.694332	0.799775	-0.695054
C	4.351148	-1.003575	-0.554705
C	3.832720	-3.211896	-0.858257
H	1.770828	-3.714928	-1.289953
C	3.697687	1.729867	-0.484489
H	1.678798	1.181389	-0.792514
C	5.347048	-0.027506	-0.309820
H	4.163278	-4.251071	-0.901348
C	5.039344	1.310169	-0.275718
H	6.368242	-0.373690	-0.159080
H	5.826022	2.038013	-0.096179
O	3.329293	3.028224	-0.506590
C	4.295845	4.006736	-0.164124
H	3.765374	4.961811	-0.177433
H	4.699016	3.829694	0.842685
H	5.114736	4.033598	-0.897071
N	-1.697154	-0.934954	-0.033818
C	-0.621362	-0.482387	3.287724
H	0.180019	0.024966	2.744373

	C	-0.640898	-0.427771	4.618688
	H	0.136766	0.092916	5.174976
	H	-1.442837	-0.892750	5.195130
	N	4.746250	-2.309220	-0.603678
	Br	-0.246840	2.645132	0.713141

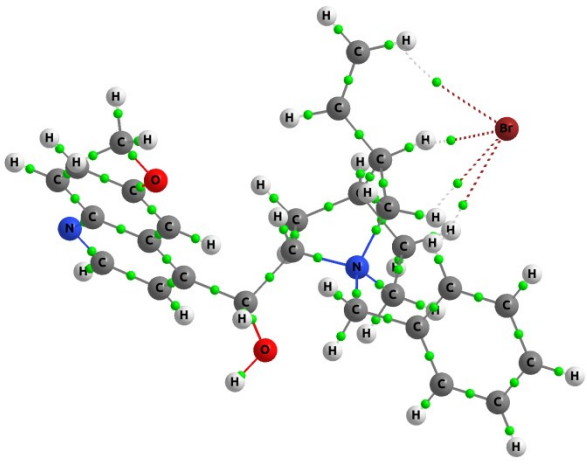
Compound	Coordinates			
	Atom	x	y	z
complex_Br_3	C	0.549698	-0.729616	-0.343165
Img. freq. = 0	C	-0.789165	-2.503673	0.802941
SCF Energy (a.u.) = -3881.67618952	C	0.557548	-2.183819	0.153993
	H	0.980402	-0.074918	0.422279
	H	0.726928	-2.863070	-0.689612
	H	1.391595	-2.306995	0.851933
	C	-1.803348	-1.258992	-1.115074
	H	-2.796327	-0.801435	-1.127785
	H	-1.420325	-1.386995	-2.127661
	C	-1.836156	-2.567681	-0.308440
	H	-2.837754	-2.693396	0.115724
	H	-1.619622	-3.410735	-0.974075
	H	-0.737008	-3.456467	1.339097
	C	-1.186641	-1.385074	1.786347
	H	-2.164045	-1.642601	2.212510
	C	-1.386811	-0.081315	0.980833
	H	-2.452346	0.160874	0.918981
	H	-0.827920	0.759157	1.406853
	C	-0.950526	1.075920	-1.174410
	H	-0.189234	1.706837	-0.700488
	H	-0.656959	0.855046	-2.204228
	C	-2.288059	1.767808	-1.163145
	C	-3.195332	1.554394	-2.204892
	C	-2.620628	2.659685	-0.139362
	C	-4.429753	2.199556	-2.208709
	H	-2.939010	0.870991	-3.014791
	C	-3.855815	3.302372	-0.138885
	H	-1.914420	2.845169	0.670030
	C	-4.763082	3.069069	-1.171731
	H	-5.136292	2.014495	-3.015782
	H	-4.114096	3.980558	0.672425
	H	-5.734137	3.561527	-1.164806
	C	1.395252	-0.525025	-1.611372
	H	1.414673	0.538879	-1.879771
	O	0.811142	-1.272184	-2.661046
	H	1.356669	-1.172356	-3.451666
	C	2.823849	-0.947380	-1.313069

	C	3.696178	-0.095947	-0.560777
	C	3.307311	-2.157671	-1.740140
	C	3.327572	1.185264	-0.085272
	C	5.008269	-0.582134	-0.290988
	C	4.638396	-2.538289	-1.421768
	H	2.679998	-2.839833	-2.310460
	C	4.217653	1.952164	0.641802
	H	2.345546	1.608637	-0.284418
	C	5.897824	0.226723	0.458687
	H	5.015380	-3.503673	-1.763089
	C	5.521932	1.463920	0.922380
	H	6.894385	-0.165399	0.654644
	H	6.226784	2.060249	1.494894
	O	3.771795	3.164070	1.052090
	C	4.661993	3.982496	1.799443
	H	4.106884	4.896073	2.024593
	H	4.954579	3.492900	2.738070
	H	5.555019	4.233784	1.211482
	N	-0.898015	-0.247288	-0.441568
	C	-0.193541	-1.212504	2.902411
	H	0.808808	-0.862574	2.633401
	C	-0.467381	-1.457146	4.183410
	H	0.284308	-1.326176	4.960627
	H	-1.457479	-1.794307	4.493197
	N	5.460278	-1.795739	-0.723435
	Br	-4.896221	-0.839908	0.887665

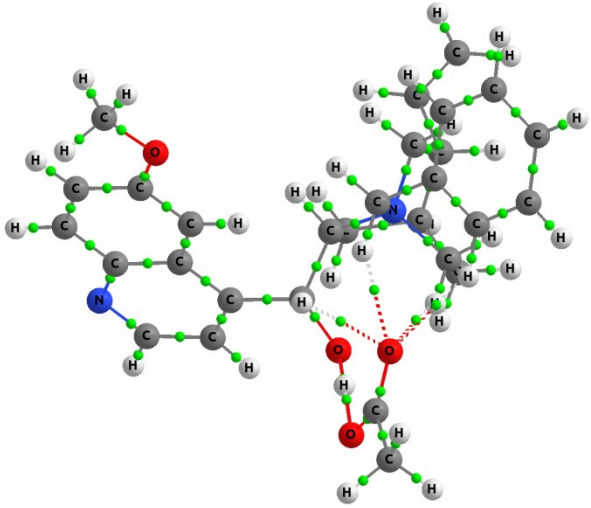
Compound	Coordinates			
	Atom	x	y	z
complex_Br_4	C	0.462899	-0.717509	0.235901
Img. freq. = 0	C	-0.757093	-1.784220	2.144496
SCF Energy (a.u.) = -3881.67116744	C	0.414785	-1.936150	1.172868
	H	1.139627	0.043159	0.639662
	H	0.283218	-2.850275	0.583139
	H	1.372977	-2.011040	1.696281
	C	-2.034967	-1.030204	0.131809
	H	-2.961088	-0.461625	0.057412
	H	-1.875867	-1.561407	-0.805765
	C	-2.054578	-1.961790	1.353655
	H	-2.925116	-1.735968	1.979007
	H	-2.156335	-2.996068	1.010374
	H	-0.683609	-2.524102	2.947621
	C	-0.753987	-0.367236	2.751672
	H	-1.592509	-0.302706	3.454978
	C	-1.025510	0.637419	1.606122

H	-2.041724	1.033783	1.655564
H	-0.319728	1.474949	1.616096
C	-0.988382	0.996419	-0.853895
H	-0.024256	1.516908	-0.855614
H	-1.098106	0.418595	-1.776276
C	-2.104948	1.998462	-0.714127
C	-3.401152	1.698070	-1.144284
C	-1.835399	3.260938	-0.171765
C	-4.421418	2.637360	-0.996901
H	-3.642083	0.724502	-1.573157
C	-2.852167	4.203052	-0.036217
H	-0.821336	3.510554	0.143141
C	-4.149954	3.887702	-0.443222
H	-5.430253	2.378478	-1.314230
H	-2.632836	5.183025	0.385148
H	-4.948489	4.620323	-0.332761
C	0.999045	-1.065142	-1.163767
H	1.007868	-0.168493	-1.796206
O	0.160025	-2.046878	-1.733886
H	0.460664	-2.234107	-2.632105
C	2.437063	-1.533081	-1.011717
C	3.490620	-0.589185	-0.786784
C	2.757548	-2.864889	-1.068370
C	3.293343	0.811788	-0.731985
C	4.806054	-1.109382	-0.617382
C	4.107211	-3.272633	-0.892709
H	1.988609	-3.615923	-1.237622
C	4.355654	1.666079	-0.507053
H	2.311769	1.259148	-0.875863
C	5.874848	-0.207832	-0.387797
H	4.355694	-4.334210	-0.936253
C	5.666822	1.148916	-0.329162
H	6.871762	-0.626749	-0.261572
H	6.507925	1.813829	-0.153599
O	4.065053	2.989475	-0.471223
C	5.134060	3.899369	-0.248358
H	4.683895	4.894728	-0.257988
H	5.606923	3.721497	0.726930
H	5.883835	3.830690	-1.047891
N	-0.901765	-0.030168	0.258477
C	0.510050	-0.047421	3.502348
H	1.433614	0.033622	2.921276
C	0.561492	0.135365	4.821147
H	1.499834	0.353011	5.328894
H	-0.337212	0.070994	5.436521

	N	5.095513	-2.442770	-0.670100
	Br	-5.315033	-1.504427	-0.796859

Compound	Coordinates			
	Atom	x	y	z
complex_Br_5	C	-0.584299	-0.906083	-0.522563
Img. freq. = 0	C	0.582897	-0.703306	-2.723864
SCF Energy (a.u.) = -3881.67166555	C	-0.739626	-1.068503	-2.042044
	H	-0.834279	0.118630	-0.230480
	H	-1.009871	-2.105334	-2.278833
	H	-1.562222	-0.429142	-2.375092
	C	1.554271	-2.154453	-0.939560
	H	2.564575	-2.245274	-0.537308
	H	0.983995	-3.053509	-0.703141
	C	1.574449	-1.835291	-2.444023
	H	2.582102	-1.537840	-2.754637
	H	1.297131	-2.736180	-3.002184
	H	0.435670	-0.572015	-3.800210
	C	1.155453	0.587171	-2.109339
	H	2.092327	0.844621	-2.616085
	C	1.541814	0.272734	-0.645322
	H	2.621760	0.156204	-0.548833
	H	1.217716	1.057889	0.043930
	C	1.095422	-1.195244	1.310465
	H	0.566271	-0.355554	1.774987
	H	0.598875	-2.133839	1.569189
	C	2.531276	-1.253546	1.769176
	C	3.090931	-2.497019	2.086181
	C	3.306026	-0.098441	1.917395
	C	4.407318	-2.589103	2.532199
	H	2.489211	-3.401028	1.984298
	C	4.627463	-0.190960	2.350327
	H	2.903389	0.882507	1.669767
	C	5.178905	-1.433473	2.660003
	H	4.831456	-3.561692	2.777405
	H	5.225778	0.714980	2.428804
	H	6.211657	-1.501910	2.999173
	C	-1.520828	-1.818036	0.286247
	H	-1.427289	-1.584285	1.355184
	O	-1.149654	-3.164446	0.055567
	H	-1.763494	-3.738559	0.531325
	C	-2.953304	-1.524869	-0.125063
	C	-3.618697	-0.343883	0.337594
	C	-3.634638	-2.368611	-0.964752
	C	-3.033980	0.593014	1.222655

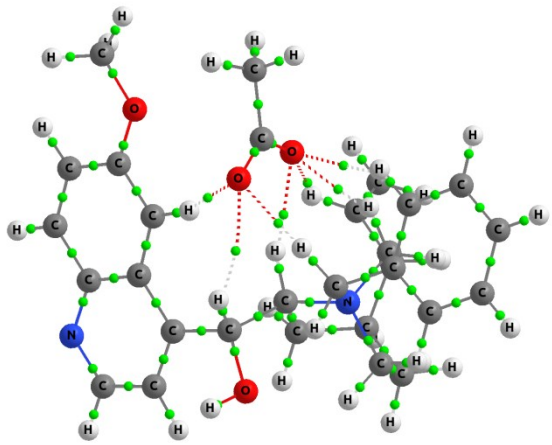
C	-4.945557	-0.118548	-0.131792
C	-4.962393	-2.052284	-1.357945
H	-3.167654	-3.273348	-1.348745
C	-3.728746	1.721299	1.615654
H	-2.032260	0.454929	1.623422
C	-5.631719	1.047591	0.288480
H	-5.498232	-2.727931	-2.026533
C	-5.046148	1.954957	1.137218
H	-6.642746	1.201503	-0.084816
H	-5.597230	2.841061	1.439497
O	-3.085988	2.557908	2.463401
C	-3.760801	3.739717	2.874758
H	-3.065465	4.263193	3.534902
H	-3.996988	4.378824	2.013524
H	-4.678459	3.498059	3.428000
N	0.901279	-1.022080	-0.180691
C	0.234117	1.772248	-2.229244
H	-0.795111	1.664619	-1.873424
C	0.621693	2.945024	-2.728912
H	-0.065530	3.787780	-2.792669
H	1.647310	3.101102	-3.065039
N	-5.598071	-0.974823	-0.971463
Br	4.188071	2.340844	-0.907589

Compound	Coordinates			
	Atom	x	y	z
complex_MeCO2_1	C	0.079341	-1.152073	-0.091252
Img. freq. = 0	C	-1.368765	-3.186493	-0.486835
SCF Energy (a.u.) = -1535.90774500	C	0.067565	-2.678125	-0.337097
	H	0.576591	-0.918973	0.854905
	H	0.616140	-2.885968	-1.259553
	H	0.583721	-3.191262	0.480859
	C	-2.219073	-0.904433	-1.074448
	H	-3.239961	-0.680647	-0.753437
	H	-1.898413	-0.164593	-1.812530
	C	-2.075012	-2.356127	-1.562633
	H	-3.069728	-2.769571	-1.763314
	H	-1.490686	-2.370542	-2.485387
	H	-1.365695	-4.246765	-0.759454
	C	-2.132204	-2.987529	0.834025
	H	-3.202029	-3.135907	0.637700
	C	-1.907498	-1.527166	1.275607
	H	-2.845036	-1.070535	1.595374
	H	-1.180727	-1.451632	2.092751
	C	-1.359052	0.772837	0.569972

H	-0.694843	0.820242	1.439460
H	-0.942991	1.327828	-0.272696
C	-2.713212	1.343181	0.911997
C	-3.487643	1.939448	-0.089922
C	-3.179727	1.345282	2.231301
C	-4.728034	2.494499	0.222850
H	-3.092464	1.984963	-1.105593
C	-4.417569	1.904121	2.544351
H	-2.565582	0.914563	3.023118
C	-5.197312	2.472821	1.536661
H	-5.324176	2.959102	-0.561170
H	-4.769945	1.903706	3.574746
H	-6.163710	2.913300	1.778929
C	0.814719	-0.402630	-1.232885
H	0.626638	0.677720	-1.166825
O	0.393541	-0.877577	-2.469885
H	0.278698	-0.065704	-3.093971
C	2.308312	-0.636205	-1.012995
C	3.033813	0.021571	0.033459
C	2.995589	-1.512515	-1.812288
C	2.461508	0.993658	0.888931
C	4.407007	-0.319505	0.200601
C	4.369914	-1.770947	-1.565974
H	2.486274	-2.001681	-2.639239
C	3.207928	1.586199	1.887856
H	1.433994	1.323522	0.758429
C	5.146917	0.304596	1.235040
H	4.904830	-2.475577	-2.205530
C	4.571048	1.233094	2.069440
H	6.194372	0.028257	1.345353
H	5.167207	1.695926	2.850980
O	2.565970	2.504140	2.657868
C	3.320791	3.177065	3.653412
H	2.630246	3.879332	4.127154
H	3.700004	2.474422	4.408527
H	4.156637	3.733715	3.207904
N	-1.361704	-0.687713	0.150540
C	-1.723604	-3.936817	1.923438
H	-0.676798	-3.903108	2.238481
C	-2.552928	-4.796998	2.513811
H	-2.207890	-5.473073	3.294777
H	-3.605454	-4.854503	2.232369
N	5.057763	-1.218047	-0.597237
C	-0.640918	2.020905	-3.438391
O	0.124271	1.147554	-3.946165

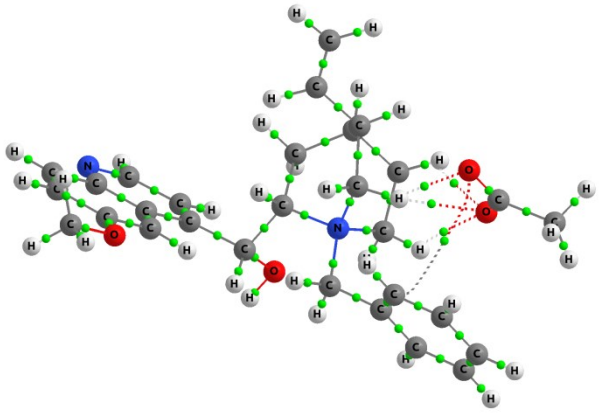
	O	-1.176589	1.939520	-2.306197
	C	-0.934734	3.239028	-4.300538
	H	-1.613809	2.936439	-5.108764
	H	-1.406557	4.031111	-3.712356
	H	-0.011790	3.602644	-4.765041

Compound	Coordinates			
	Atom	x	y	z
complex_MeCO2_2	C	-0.130080	-1.181003	0.020979
Img. freq. = 0	C	-0.917199	-2.629043	1.903280
SCF Energy (a.u.) = -1535.89511367	C	0.229201	-2.367797	0.926034
	H	0.196735	-0.228629	0.455062
	H	0.408597	-3.264556	0.319750
	H	1.160276	-2.132279	1.451161
	C	-2.338100	-2.376621	-0.132612
	H	-3.401477	-2.160368	-0.257435
	H	-1.949510	-2.827573	-1.044708
	C	-2.077284	-3.240643	1.114144
	H	-2.975590	-3.292272	1.740785
	H	-1.828422	-4.259909	0.798995
	H	-0.593552	-3.298441	2.706715
	C	-1.405178	-1.295889	2.502025
	H	-2.188991	-1.527628	3.233967
	C	-2.046843	-0.474248	1.361273
	H	-3.137482	-0.522179	1.398932
	H	-1.710725	0.566189	1.366471
	C	-2.074596	-0.098186	-1.107334
	H	-1.361486	0.736806	-1.089463
	H	-1.951755	-0.672752	-2.029832
	C	-3.479452	0.432337	-0.990312
	C	-4.563446	-0.229467	-1.575831
	C	-3.698021	1.649056	-0.332798
	C	-5.852194	0.295209	-1.477366
	H	-4.397945	-1.155500	-2.127424
	C	-4.984452	2.174272	-0.232337
	H	-2.846849	2.180071	0.095530
	C	-6.064539	1.494924	-0.798733
	H	-6.688711	-0.226697	-1.939971
	H	-5.143788	3.121762	0.280245
	H	-7.069612	1.908278	-0.724164
	C	0.524383	-1.255456	-1.372033
	H	0.389165	-0.288792	-1.876871
	O	-0.099604	-2.291360	-2.118694
	H	0.312045	-2.320031	-2.991545
	C	2.015273	-1.517359	-1.198254



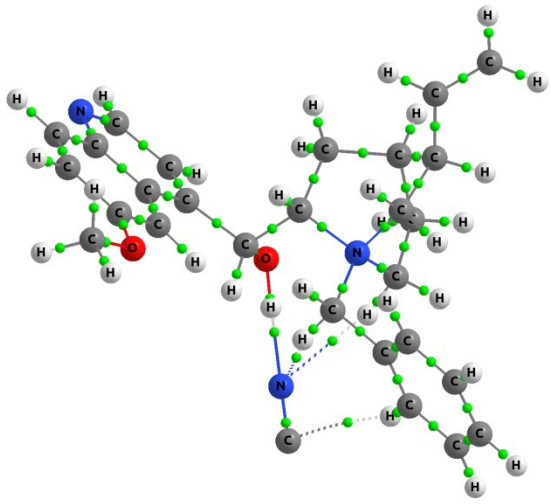
	C	2.907277	-0.484331	-0.762921
	C	2.536168	-2.767481	-1.420844
	C	2.495137	0.847090	-0.539126
	C	4.272738	-0.843590	-0.553350
	C	3.918402	-3.009637	-1.199898
	H	1.900712	-3.588163	-1.746274
	C	3.403739	1.792861	-0.102133
	H	1.473822	1.174217	-0.727726
	C	5.175000	0.147667	-0.099288
	H	4.321199	-4.008343	-1.378633
	C	4.759288	1.438380	0.130112
	H	6.211853	-0.144110	0.059337
	H	5.476318	2.177385	0.477137
	O	2.922822	3.047465	0.072560
	C	3.810582	4.042762	0.549222
	H	3.219053	4.958761	0.623112
	H	4.203474	3.782955	1.542377
	H	4.642437	4.204500	-0.150837
	N	-1.657571	-1.039714	0.009501
	C	-0.314764	-0.532668	3.208975
	H	0.374535	0.046766	2.589246
	C	-0.173888	-0.519008	4.533966
	H	0.630535	0.036888	5.012674
	H	-0.865095	-1.057640	5.184973
	N	4.759520	-2.101384	-0.773684
	C	-0.218868	2.763403	-0.152614
	O	-0.328675	1.987896	0.839437
	O	-0.220469	2.395705	-1.356370
	C	-0.109061	4.257810	0.131904
	H	0.459256	4.756031	-0.659641
	H	-1.121513	4.685789	0.146975
	H	0.350919	4.429422	1.110104

Compound	Coordinates			
	Atom	x	y	z
complex_MeCO2_3	C	0.546792	-0.852678	-0.220794
Img. freq. = 0	C	-0.686855	-2.496018	1.213237
SCF Energy (a.u.) = -1535.88324191	C	0.631488	-2.215840	0.485820
	H	0.932982	-0.068175	0.439393
	H	0.815469	-3.004256	-0.254052
	H	1.484772	-2.199258	1.170925
	C	-1.746459	-1.658531	-0.888071
	H	-2.760293	-1.276008	-1.016031
	H	-1.302974	-1.953178	-1.839574
	C	-1.751014	-2.786265	0.154935



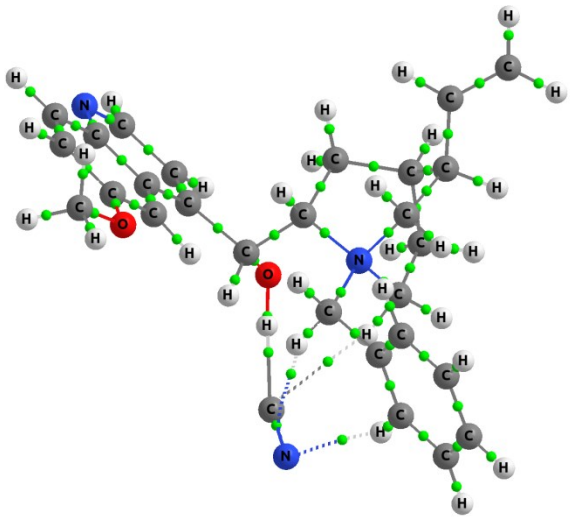
H	-2.744679	-2.828088	0.612476
H	-1.540334	-3.740525	-0.341094
H	-0.571448	-3.345225	1.894427
C	-1.133052	-1.252866	2.006118
H	-2.089640	-1.473920	2.494892
C	-1.425735	-0.122964	0.995411
H	-2.504349	0.027957	0.924818
H	-0.926113	0.812400	1.268726
C	-1.083668	0.693473	-1.316993
H	-0.410214	1.469113	-0.932814
H	-0.733197	0.353552	-2.295602
C	-2.492443	1.215658	-1.443482
C	-3.287474	0.797452	-2.514939
C	-3.014839	2.126515	-0.521967
C	-4.592900	1.261478	-2.651235
H	-2.883034	0.092933	-3.242372
C	-4.322094	2.588311	-0.652460
H	-2.409316	2.464818	0.317324
C	-5.113761	2.154226	-1.714943
H	-5.206302	0.920499	-3.483624
H	-4.725640	3.278101	0.086451
H	-6.139646	2.507600	-1.809999
C	1.394214	-0.780978	-1.502229
H	1.348241	0.234557	-1.917331
O	0.875946	-1.705322	-2.439673
H	1.431799	-1.686648	-3.229091
C	2.843109	-1.064230	-1.143527
C	3.661288	-0.053427	-0.543049
C	3.399014	-2.296817	-1.374320
C	3.215590	1.263166	-0.275816
C	5.000080	-0.411778	-0.210104
C	4.748631	-2.543166	-1.007007
H	2.814854	-3.096191	-1.825781
C	4.058814	2.189072	0.308126
H	2.209407	1.588479	-0.530485
C	5.840038	0.559217	0.388817
H	5.182517	-3.527581	-1.189796
C	5.390790	1.830952	0.648698
H	6.858619	0.264360	0.635419
H	6.060395	2.553631	1.106096
O	3.542367	3.423216	0.522080
C	4.381040	4.401591	1.122118
H	3.772591	5.305434	1.201350
H	4.699924	4.087494	2.125267
H	5.259239	4.606995	0.495119

N	-0.925551	-0.487450	-0.386168
C	-0.138714	-0.840775	3.055894
H	0.857694	-0.539823	2.715754
C	-0.406101	-0.814127	4.361160
H	0.344197	-0.509482	5.089552
H	-1.391999	-1.088177	4.738758
N	5.524055	-1.650604	-0.444184
C	-4.875344	-0.174633	1.214531
O	-4.259694	0.375772	2.161788
O	-4.388691	-1.012422	0.404680
C	-6.358083	0.174878	1.047841
H	-6.698015	-0.028891	0.026813
H	-6.938068	-0.453092	1.738536
H	-6.540496	1.221644	1.316382

Compound	Coordinates			
	Atom	x	y	z
complex_CN_1	C	-0.062407	-0.963641	-0.050081
Img. freq. = 0	C	1.249348	-2.999008	-0.772875
SCF Energy (a.u.) = -1400.23261422	C	-0.149382	-2.420782	-0.556495
	H	-0.521481	-0.280009	-0.770429
	H	-0.665946	-3.024585	0.195268
	H	-0.743698	-2.456107	-1.475036
	C	2.275723	-1.384855	0.834634
	H	3.301982	-1.093041	0.596075
	H	2.060551	-1.106299	1.867752
	C	2.021844	-2.870877	0.542393
	H	2.982194	-3.393498	0.476204
	H	1.438959	-3.308898	1.357439
	H	1.179162	-4.047928	-1.078145
	C	1.995752	-2.191415	-1.849572
	H	3.053416	-2.484064	-1.825582
	C	1.888133	-0.697465	-1.474379
	H	2.858533	-0.205780	-1.550648
	H	1.171022	-0.165808	-2.109376
	C	1.501565	0.935605	0.353277
	H	0.792546	1.464122	-0.292966
	H	1.174043	0.980449	1.394387
	C	2.876354	1.545330	0.239437
	C	3.761273	1.479775	1.321069
	C	3.256906	2.238209	-0.915514
	C	5.020951	2.070719	1.233089
	H	3.450949	0.987607	2.243194
	C	4.514816	2.830743	-1.003389
	H	2.558853	2.323285	-1.749380

C	5.401545	2.740917	0.070462
H	5.699186	2.020766	2.083341
H	4.799670	3.371298	-1.904814
H	6.383307	3.208411	0.006601
C	-0.786045	-0.786823	1.308077
H	-0.621078	0.224997	1.702133
O	-0.346904	-1.730134	2.240112
H	0.163850	-1.213750	2.925002
C	-2.275565	-0.937404	1.035609
C	-3.018305	0.082033	0.356502
C	-2.941556	-2.074065	1.414421
C	-2.466956	1.328198	-0.028235
C	-4.390615	-0.180521	0.077951
C	-4.316718	-2.227730	1.095915
H	-2.419231	-2.853812	1.963535
C	-3.234898	2.268586	-0.685921
H	-1.439290	1.590492	0.213464
C	-5.151945	0.802836	-0.600944
H	-4.836980	-3.139284	1.395556
C	-4.597484	2.000746	-0.983183
H	-6.198258	0.580792	-0.804694
H	-5.209584	2.736484	-1.497183
O	-2.615603	3.431431	-1.015199
C	-3.391379	4.440435	-1.644516
H	-2.714523	5.284748	-1.796444
H	-3.772808	4.099675	-2.617088
H	-4.226485	4.754610	-1.003807
N	1.407875	-0.524901	-0.056053
C	1.479414	-2.420887	-3.241098
H	0.429963	-2.172264	-3.423492
C	2.219325	-2.897334	-4.241736
H	1.798956	-3.053514	-5.234170
H	3.271482	-3.148323	-4.099541
N	-5.020982	-1.335821	0.443553
C	1.703485	0.811441	4.225831
N	1.070495	-0.028955	3.705238

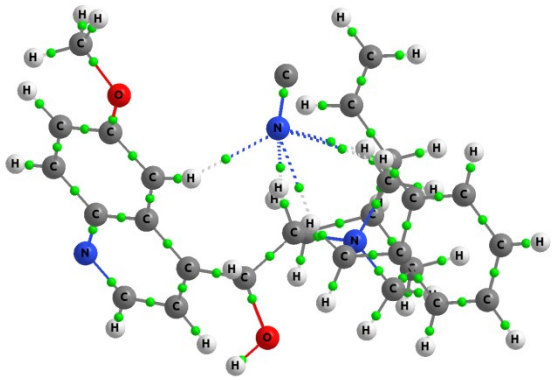
Compound	Coordinates			
	Atom	x	y	z
complex_NC_1	C	-0.065288	-0.987915	-0.035964
Img. freq. = 0	C	1.267037	-3.028413	-0.704596
SCF Energy (a.u.) = -1400.23138843	C	-0.137725	-2.454521	-0.517220
	H	-0.525542	-0.319773	-0.770083
	H	-0.661272	-3.047179	0.238385
	H	-0.718514	-2.510187	-1.443410



C	2.266504	-1.370141	0.876688
H	3.293427	-1.072890	0.646940
H	2.034636	-1.074087	1.901264
C	2.027781	-2.864345	0.613750
H	2.992842	-3.380213	0.566048
H	1.441814	-3.289287	1.433418
H	1.206642	-4.084784	-0.985519
C	2.016696	-2.241168	-1.793498
H	3.075911	-2.526673	-1.755366
C	1.897908	-0.740279	-1.451342
H	2.867282	-0.246691	-1.527660
H	1.185109	-0.225299	-2.104731
C	1.481912	0.933753	0.330436
H	0.769074	1.437795	-0.330810
H	1.152320	1.005672	1.369244
C	2.849739	1.555912	0.202424
C	3.727650	1.541701	1.291747
C	3.228191	2.210738	-0.975362
C	4.981376	2.143364	1.187128
H	3.412415	1.088143	2.232293
C	4.479661	2.813965	-1.078791
H	2.534017	2.257261	-1.815442
C	5.361559	2.773489	0.002269
H	5.655236	2.133515	2.042367
H	4.763176	3.324710	-1.997881
H	6.338502	3.249220	-0.074144
C	-0.799424	-0.796233	1.315167
H	-0.632284	0.218761	1.702306
O	-0.374231	-1.734796	2.256786
H	0.083338	-1.211560	2.984901
C	-2.288517	-0.939340	1.029605
C	-3.023076	0.081657	0.343649
C	-2.961831	-2.072755	1.405409
C	-2.465096	1.325275	-0.039860
C	-4.394834	-0.175949	0.057166
C	-4.335156	-2.222331	1.077427
H	-2.446090	-2.853434	1.959459
C	-3.226093	2.268216	-0.701991
H	-1.438137	1.584463	0.207228
C	-5.148797	0.809761	-0.626487
H	-4.860453	-3.131912	1.374328
C	-4.588026	2.005476	-1.006316
H	-6.194770	0.591338	-0.835806
H	-5.194604	2.743328	-1.523841
O	-2.600788	3.428588	-1.028682

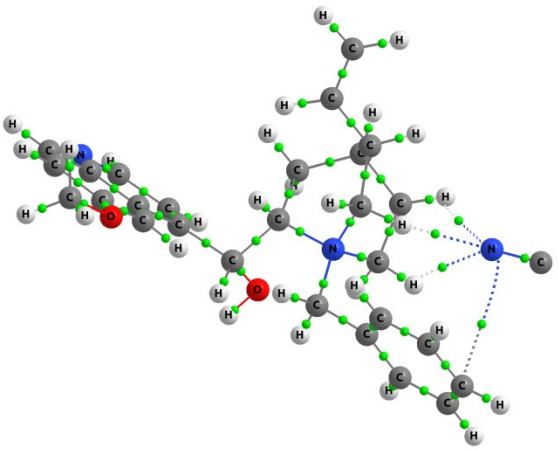
	C	-3.371550	4.442517	-1.656153
	H	-2.691666	5.285345	-1.802603
	H	-3.751231	4.106992	-2.631243
	H	-4.207547	4.756621	-1.016560
	N	1.402235	-0.537889	-0.041942
	C	1.512019	-2.504785	-3.183341
	H	0.463982	-2.261546	-3.380609
	C	2.260636	-3.005339	-4.165587
	H	1.848563	-3.186686	-5.157233
	H	3.311807	-3.251617	-4.008530
	N	-5.031955	-1.328505	0.419764
	N	1.804061	0.883198	4.039997
	C	1.025370	0.034805	3.829265

Compound	Coordinates			
	Atom	x	y	z
complex_CN_2	C	-0.174475	-0.904115	0.092908
Img. freq. = 0	C	-1.065168	-2.217782	2.027313
SCF Energy (a.u.) = -1400.22043720	C	0.117482	-2.049326	1.072762
	H	0.183993	0.053648	0.486329
	H	0.281618	-2.984388	0.522681
	H	1.041350	-1.814598	1.610363
	C	-2.425397	-2.027342	-0.055950
	H	-3.476976	-1.775584	-0.206794
	H	-2.043190	-2.538618	-0.938642
	C	-2.218994	-2.836909	1.236589
	H	-3.134947	-2.836560	1.838841
	H	-1.988161	-3.875727	0.976586
	H	-0.787325	-2.852188	2.874888
	C	-1.527735	-0.840833	2.540577
	H	-2.348501	-1.009472	3.248775
	C	-2.097032	-0.054053	1.336508
	H	-3.189335	-0.049018	1.344936
	H	-1.724379	0.972907	1.299134
	C	-2.056565	0.179535	-1.149742
	H	-1.364409	1.024240	-1.088736
	H	-1.862252	-0.425636	-2.039153
	C	-3.476420	0.684369	-1.148050
	C	-4.495425	-0.019610	-1.798780
	C	-3.771189	1.910349	-0.539689
	C	-5.798836	0.475588	-1.814280
	H	-4.266398	-0.954262	-2.312114
	C	-5.074180	2.404858	-0.553662
	H	-2.969064	2.477651	-0.065214
	C	-6.090364	1.685872	-1.184604



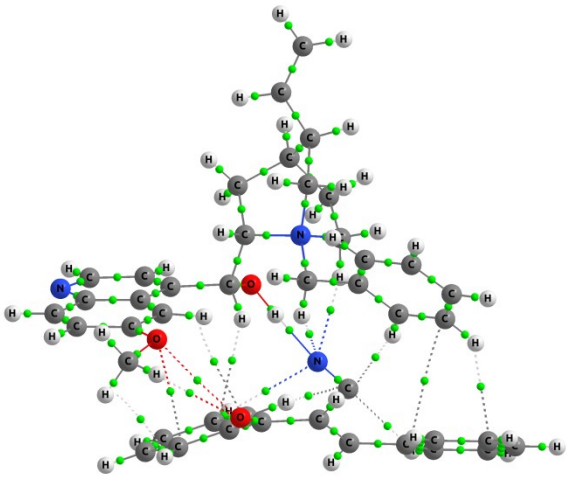
	H	-6.584854	-0.077427	-2.326561
	H	-5.293158	3.360009	-0.078821
	H	-7.107340	2.076018	-1.198719
	C	0.507046	-1.078310	-1.276379
	H	0.415954	-0.139539	-1.839235
	O	-0.144569	-2.128929	-1.975913
	H	0.312183	-2.258909	-2.816743
	C	1.986486	-1.377355	-1.075570
	C	2.930174	-0.343614	-0.767261
	C	2.448634	-2.665641	-1.187304
	C	2.588140	1.023634	-0.649138
	C	4.289274	-0.743443	-0.580755
	C	3.824659	-2.947654	-0.985799
	H	1.770414	-3.483986	-1.419167
	C	3.563297	1.963420	-0.362177
	H	1.566361	1.387064	-0.755246
	C	5.256775	0.242199	-0.269808
	H	4.180047	-3.975820	-1.073892
	C	4.912766	1.566997	-0.158982
	H	6.285065	-0.085597	-0.126431
	H	5.677246	2.302774	0.075502
	O	3.158922	3.250175	-0.305049
	C	4.086304	4.227954	0.135171
	H	3.525249	5.164132	0.184836
	H	4.473597	3.983971	1.134018
	H	4.918763	4.337445	-0.574214
	N	-1.696381	-0.709791	0.029343
	C	-0.442136	-0.084713	3.260360
	H	0.338043	0.381909	2.653474
	C	-0.403674	0.054465	4.584598
	H	0.397919	0.606378	5.072256
	H	-1.181420	-0.368242	5.223298
	N	4.716053	-2.036011	-0.689210
	C	-0.260143	3.185287	1.170471
	N	-0.299777	2.449302	0.254936

Compound	Coordinates			
	Atom	x	y	z
complex_CN_3	C	0.141469	-0.844085	-0.155317
Img. freq. = 0	C	-1.017932	-2.500747	1.320229
SCF Energy (a.u.) = -1400.21353201	C	0.248736	-2.227589	0.506089
	H	0.591132	-0.085275	0.493987
	H	0.361710	-2.998335	-0.265674
	H	1.148867	-2.246289	1.128034
	C	-2.214799	-1.581687	-0.670612



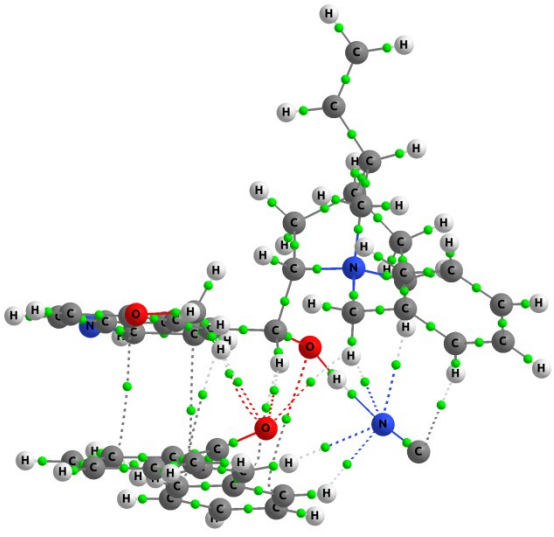
H	-3.225568	-1.173643	-0.719357
H	-1.852871	-1.859514	-1.660800
C	-2.165944	-2.738117	0.339437
H	-3.121462	-2.783878	0.872721
H	-2.015637	-3.681210	-0.197354
H	-0.873584	-3.369463	1.970165
C	-1.373892	-1.270549	2.177067
H	-2.285971	-1.506133	2.738760
C	-1.725892	-0.107938	1.220146
H	-2.807043	0.052962	1.204295
H	-1.196118	0.814561	1.480272
C	-1.520364	0.767224	-1.096153
H	-0.783995	1.504643	-0.755803
H	-1.269822	0.432937	-2.106473
C	-2.909438	1.347175	-1.079956
C	-3.846671	0.932251	-2.030194
C	-3.278289	2.301029	-0.127115
C	-5.148575	1.423763	-1.997893
H	-3.561653	0.201427	-2.787345
C	-4.580617	2.791041	-0.090892
H	-2.550024	2.647807	0.605820
C	-5.519295	2.343006	-1.018860
H	-5.879772	1.074279	-2.724368
H	-4.868466	3.512054	0.672001
H	-6.544730	2.705747	-0.973668
C	0.894288	-0.757890	-1.493712
H	0.826620	0.262479	-1.892489
O	0.302649	-1.666268	-2.402545
H	0.787147	-1.627140	-3.236986
C	2.362229	-1.055121	-1.237579
C	3.219013	-0.064758	-0.656902
C	2.897766	-2.281471	-1.537672
C	2.796839	1.245409	-0.326844
C	4.572110	-0.437599	-0.409733
C	4.265801	-2.542123	-1.257769
H	2.284746	-3.065831	-1.976834
C	3.675101	2.149330	0.239628
H	1.781494	1.584941	-0.518419
C	5.448395	0.510749	0.173690
H	4.684390	-3.521029	-1.496754
C	5.021073	1.775276	0.498265
H	6.477100	0.204063	0.355269
H	5.718075	2.479612	0.943561
O	3.175900	3.377525	0.518872
C	4.052019	4.339220	1.092073

	H	3.453845	5.243868	1.223714
	H	4.423391	4.002464	2.069369
	H	4.895511	4.553646	0.421989
	N	-1.331058	-0.442497	-0.203349
	C	-0.290804	-0.905689	3.154402
	H	0.665234	-0.565184	2.744566
	C	-0.431865	-0.975592	4.477732
	H	0.381945	-0.710348	5.150980
	H	-1.370669	-1.299953	4.928808
	N	5.075834	-1.670150	-0.711740
	C	-5.994874	-0.733569	1.109990
	N	-4.824170	-0.727356	1.007676

Compound	Coordinates			
	Atom	x	y	z
preTS_cat1_R	C	-1.822787	1.841277	-0.178943
Img. freq. = 0	C	-1.895491	4.345122	-0.520153
SCF Energy (a.u.) = -2054.05178949	C	-2.732017	3.066266	-0.422186
	H	-2.088513	1.342338	0.757220
	H	-3.270245	2.920916	-1.362017
	H	-3.476128	3.143226	0.375477
	C	0.182011	3.078408	-1.098906
	H	1.112223	3.521680	-0.735575
	H	0.423474	2.335721	-1.861594
	C	-0.816712	4.139014	-1.587519
	H	-0.283766	5.075303	-1.777028
	H	-1.276945	3.804083	-2.518432
	H	-2.534911	5.193303	-0.778942
	C	-1.188362	4.615282	0.820697
	H	-0.425760	5.385097	0.652543
	C	-0.484879	3.308435	1.245219
	H	0.531440	3.503087	1.587053
	H	-1.027314	2.788431	2.041772
	C	0.492711	1.157263	0.471540
	H	-0.036321	0.651293	1.284845
	H	0.521656	0.512319	-0.408295
	C	1.901500	1.493684	0.886223
	C	2.927913	1.473858	-0.062516
	C	2.213737	1.726118	2.230170
	C	4.242080	1.722406	0.325786
	H	2.702871	1.220234	-1.098065
	C	3.527030	1.974023	2.616492
	H	1.425770	1.693741	2.979844
	C	4.541805	1.978076	1.661253
	H	5.035617	1.681256	-0.414916

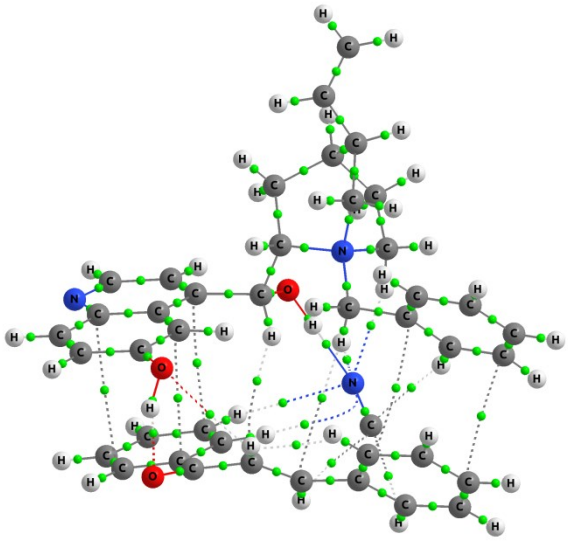
H	3.758662	2.148970	3.662703
H	5.570359	2.157736	1.960512
C	-1.937769	0.810928	-1.331725
H	-1.144724	0.057560	-1.247287
O	-1.856192	1.439452	-2.575463
H	-1.021986	1.085663	-2.994993
C	-3.263167	0.080494	-1.170500
C	-3.449823	-0.893593	-0.139217
C	-4.309741	0.331812	-2.017140
C	-2.430198	-1.286162	0.752352
C	-4.725318	-1.518537	-0.045553
C	-5.542737	-0.345106	-1.828388
H	-4.187312	1.034632	-2.833895
C	-2.653674	-2.248167	1.714213
H	-1.424089	-0.894051	0.669285
C	-4.930265	-2.499867	0.955464
H	-6.374833	-0.131798	-2.497455
C	-3.928220	-2.862126	1.821706
H	-5.911515	-2.961083	1.012305
H	-4.113816	-3.617713	2.576727
O	-1.601715	-2.545957	2.509955
N	-0.391603	2.337797	0.090807
C	-2.106632	5.102260	1.906476
H	-2.911269	4.428554	2.205028
C	-1.989293	6.285955	2.500191
H	-2.682034	6.608762	3.271528
H	-1.194424	6.978914	2.232541
N	-5.761280	-1.227417	-0.885093
C	-1.654513	-3.564547	-1.832623
C	-0.736104	-2.535052	-2.013017
C	0.299153	-2.356216	-1.096931
C	0.430765	-3.213697	-0.000905
C	-0.495328	-4.249617	0.169710
C	-1.531666	-4.424122	-0.738638
H	-2.468498	-3.697530	-2.539397
H	-0.810245	-1.854902	-2.857694
H	0.990618	-1.535601	-1.256072
H	-0.385351	-4.905522	1.028228
H	-2.250260	-5.225933	-0.595105
C	1.473350	-3.023651	1.058613
O	1.306563	-3.497351	2.173528
C	2.723813	-2.265232	0.792169
H	3.195087	-1.879208	1.694640
C	3.335260	-2.148351	-0.397119
H	2.859181	-2.541073	-1.293265

	C	4.643593	-1.509454	-0.612412
	C	5.614725	-1.436485	0.394439
	C	4.919866	-0.947553	-1.866183
	C	6.829936	-0.804542	0.156224
	H	5.424017	-1.895105	1.360643
	C	6.135717	-0.312070	-2.101020
	H	4.151012	-0.970768	-2.634952
	C	7.094700	-0.240508	-1.091788
	H	7.578530	-0.761601	0.942208
	H	6.332620	0.127256	-3.074539
	H	8.048199	0.245432	-1.277656
	C	1.660924	0.042851	-3.068060
	N	0.547754	0.411549	-3.139441
	C	-1.699358	-3.673362	3.358586
	H	-0.700825	-3.821810	3.767458
	H	-2.415665	-3.499632	4.171294
	H	-1.997130	-4.567919	2.798775

Compound	Coordinates			
	Atom	x	y	z
preTS_cat1_S	C	-1.514937	0.952055	-1.029907
Img. freq. = 0	C	-3.468542	2.423944	-1.651032
SCF Energy (a.u.) = -2054.05387702	C	-1.998158	2.109931	-1.928158
	H	-1.254091	0.084232	-1.640685
	H	-1.400131	2.998189	-1.708015
	H	-1.834420	1.854452	-2.978826
	C	-3.335079	1.501991	0.668240
	H	-4.261545	1.052686	1.033095
	H	-2.677424	1.678463	1.519072
	C	-3.599460	2.764634	-0.163930
	H	-4.601651	3.140852	0.060716
	H	-2.871141	3.534033	0.101675
	H	-3.796942	3.263613	-2.269443
	C	-4.344108	1.190300	-1.946864
	H	-5.346525	1.385168	-1.547640
	C	-3.740600	-0.017560	-1.191263
	H	-4.508473	-0.556806	-0.637577
	H	-3.243385	-0.719283	-1.868807
	C	-2.234209	-0.738788	0.668910
	H	-1.682218	-1.400064	-0.006342
	H	-1.545373	-0.324511	1.408435
	C	-3.336930	-1.491957	1.366955
	C	-3.727005	-1.119051	2.656538
	C	-3.937356	-2.602680	0.764384
	C	-4.728318	-1.828219	3.315709

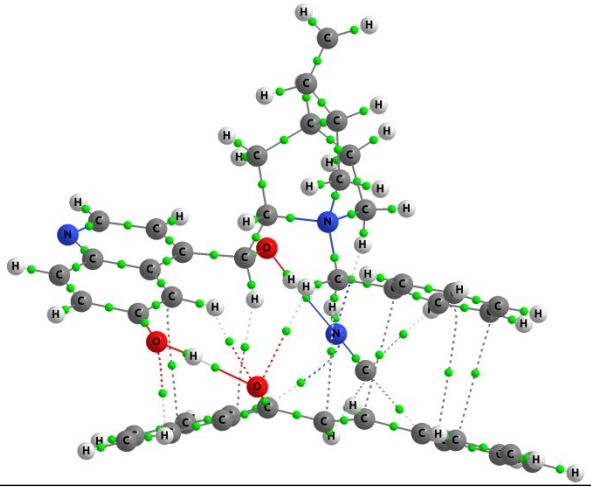
H	-3.218651	-0.296322	3.155705
C	-4.937096	-3.310505	1.423775
H	-3.612643	-2.918723	-0.225344
C	-5.338583	-2.917712	2.699353
H	-5.019395	-1.534958	4.319400
H	-5.395253	-4.171683	0.947241
H	-6.115634	-3.471235	3.217790
C	-0.282862	1.355175	-0.186966
H	-0.023971	0.541977	0.506864
O	-0.538977	2.537653	0.507256
H	-0.619082	2.298611	1.476813
C	0.903662	1.532953	-1.127731
C	1.513336	0.425567	-1.793738
C	1.438096	2.780248	-1.330276
C	1.098416	-0.921207	-1.605626
C	2.618632	0.696471	-2.643862
C	2.540979	2.936526	-2.203676
H	1.031031	3.632630	-0.798060
C	1.746338	-1.950069	-2.249664
H	0.313720	-1.140132	-0.894605
C	3.258914	-0.390842	-3.304811
H	2.959424	3.929108	-2.361331
C	2.837921	-1.676989	-3.119631
H	4.097106	-0.157723	-3.954087
H	3.323179	-2.515554	-3.608916
O	1.432966	-3.257607	-2.110434
N	-2.698644	0.430866	-0.195407
C	-4.477589	0.886092	-3.413044
H	-3.556831	0.638701	-3.943417
C	-5.629724	0.906758	-4.076032
H	-5.678598	0.693660	-5.139567
H	-6.567758	1.141902	-3.577820
N	3.115814	1.948224	-2.847831
C	4.068224	-5.076020	0.184944
C	4.532224	-3.850677	-0.286558
C	3.901405	-2.670436	0.096510
C	2.786023	-2.711890	0.938725
C	2.318513	-3.948033	1.398986
C	2.961426	-5.123835	1.032369
H	4.567818	-5.994551	-0.108349
H	5.386084	-3.811983	-0.956030
H	4.259464	-1.725177	-0.299463
H	1.447508	-3.965246	2.047361
H	2.601125	-6.077942	1.404873
C	2.025933	-1.480866	1.333092

O	0.836474	-1.572993	1.624439
C	2.737029	-0.187681	1.354979
H	3.730929	-0.135945	0.923308
C	2.166736	0.883466	1.934139
H	1.200904	0.744965	2.422875
C	2.710908	2.243250	1.973033
C	2.072179	3.195041	2.779681
C	3.810439	2.639855	1.195721
C	2.536020	4.506388	2.826504
H	1.202621	2.893864	3.358745
C	4.268834	3.949277	1.240979
H	4.290956	1.926889	0.531167
C	3.634904	4.885598	2.060300
H	2.033831	5.233189	3.457599
H	5.116802	4.245406	0.630603
H	3.994251	5.909975	2.092187
C	-1.286585	1.099735	3.973414
N	-0.943828	1.588956	2.960477
C	0.286974	-3.570839	-1.340135
H	0.369885	-3.195087	-0.314399
H	-0.617329	-3.159506	-1.811891
H	0.223178	-4.659253	-1.321688

Compound	Coordinates			
	Atom	x	y	z
preTS_cat2_R	C	0.009390	2.267109	-0.027244
Img. freq. = 0	C	1.162179	4.421720	-0.670003
SCF Energy (a.u.) = -2014.76609212	C	-0.166717	3.783615	-0.262596
	H	-0.234189	2.010428	1.007101
	H	-0.893307	3.931414	-1.065694
	H	-0.572114	4.254747	0.637219
	C	2.078490	2.244073	-1.493744
	H	3.158230	2.120128	-1.383357
	H	1.708194	1.491522	-2.191316
	C	1.697612	3.677068	-1.896219
	H	2.579626	4.184693	-2.297615
	H	0.929889	3.643456	-2.671481
	H	1.015427	5.481097	-0.897387
	C	2.188696	4.272342	0.468559
	H	3.175204	4.540199	0.071644
	C	2.212210	2.784942	0.886454
	H	3.234923	2.419162	0.967371
	H	1.704570	2.616415	1.841780
	C	1.720519	0.442632	0.201097
	H	1.232896	0.286380	1.168563

H	1.201265	-0.124850	-0.574459
C	3.161858	0.004604	0.249484
C	3.760242	-0.529246	-0.895975
C	3.896030	0.071456	1.438302
C	5.092554	-0.933541	-0.862997
H	3.169360	-0.650804	-1.802159
C	5.226763	-0.334230	1.469859
H	3.420823	0.439909	2.345215
C	5.830054	-0.824382	0.313476
H	5.547000	-1.351027	-1.756278
H	5.788775	-0.274835	2.397037
H	6.868324	-1.142409	0.335871
C	-0.889612	1.440152	-0.971405
H	-0.637588	0.375022	-0.888936
O	-0.727587	1.862899	-2.292783
H	-0.332419	1.078584	-2.772378
C	-2.340691	1.570134	-0.532205
C	-2.829134	0.911588	0.636055
C	-3.235934	2.258575	-1.310473
C	-2.016398	0.128741	1.497602
C	-4.225657	0.986090	0.895711
C	-4.600897	2.294476	-0.939582
H	-2.901555	2.730674	-2.227434
C	-2.562779	-0.541219	2.563024
H	-0.960186	-0.018706	1.297282
C	-4.761652	0.278589	2.006173
H	-5.308260	2.845272	-1.557776
C	-3.954582	-0.464992	2.823591
H	-5.832194	0.347439	2.172809
H	-4.359466	-1.013254	3.669413
O	-1.752258	-1.297680	3.364167
N	1.505390	1.918266	-0.128865
C	1.909609	5.152017	1.655012
H	0.966971	4.979489	2.176497
C	2.731742	6.104078	2.085305
H	2.483758	6.725217	2.940680
H	3.683229	6.298684	1.594990
N	-5.094145	1.682579	0.110542
H	-2.097806	-2.210738	3.336558
C	-4.361912	-1.140788	-2.269761
C	-2.972706	-1.161606	-2.371307
C	-2.212927	-1.808678	-1.402171
C	-2.837616	-2.456638	-0.330438
C	-4.235312	-2.439089	-0.240728
C	-4.992336	-1.783598	-1.203630

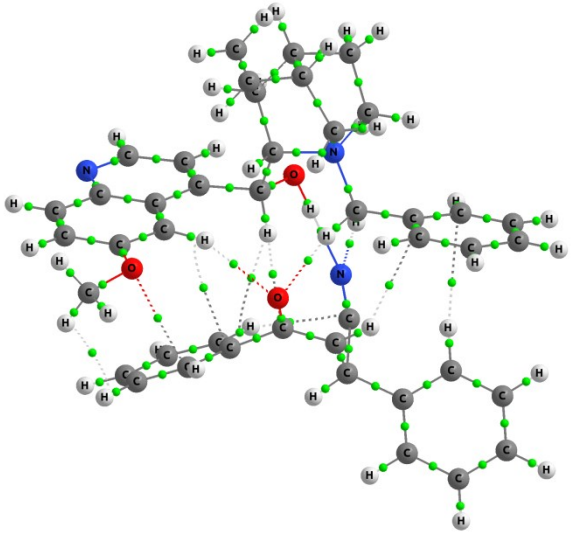
	H	-4.954205	-0.615198	-3.013399
	H	-2.463033	-0.655118	-3.186555
	H	-1.133864	-1.767581	-1.489701
	H	-4.708893	-2.923701	0.606558
	H	-6.074389	-1.757908	-1.116016
	C	-2.083758	-3.034349	0.823378
	O	-2.693296	-3.390739	1.831026
	C	-0.603176	-3.114555	0.857532
	H	-0.215684	-3.029085	1.870358
	C	0.213959	-3.422254	-0.163754
	H	-0.197953	-3.573894	-1.159213
	C	1.666157	-3.636468	-0.062548
	C	2.386298	-3.439349	1.125323
	C	2.357384	-4.064116	-1.203689
	C	3.752128	-3.684639	1.172760
	H	1.879023	-3.093892	2.021814
	C	3.724025	-4.317968	-1.153436
	H	1.815044	-4.178147	-2.137081
	C	4.423886	-4.133595	0.035313
	H	4.296345	-3.521765	2.098343
	H	4.242357	-4.653540	-2.046745
	H	5.492329	-4.325954	0.075838
	C	0.909476	-1.474701	-2.982262
	N	0.489312	-0.377612	-3.033716

Compound	Coordinates			
	Atom	x	y	z
preTS_cat2_S	C	-1.380821	1.805474	-0.254795
Img. freq. = 0	C	-1.259649	4.273282	-0.782699
SCF Energy (a.u.) = -2014.78051367	C	-2.192819	3.086208	-0.549090
	H	-1.575792	1.456315	0.762591
	H	-2.788334	2.926271	-1.451569
	H	-2.889168	3.278291	0.271849
	C	0.606799	2.777496	-1.505875
	H	1.608640	3.146725	-1.277097
	H	0.685688	1.976628	-2.241278
	C	-0.330033	3.911355	-1.943844
	H	0.267528	4.776967	-2.244253
	H	-0.922832	3.584880	-2.801372
	H	-1.841731	5.167467	-1.021350
	C	-0.401320	4.533365	0.469613
	H	0.383296	5.250332	0.199365
	C	0.266546	3.199647	0.874307
	H	1.334399	3.329326	1.048576
	H	-0.182734	2.770685	1.776033

C	0.931174	0.917171	0.127475
H	0.440219	0.462501	0.994848
H	0.848773	0.253058	-0.736626
C	2.385441	1.183297	0.419932
C	3.316342	1.234047	-0.621156
C	2.829350	1.318480	1.740107
C	4.662972	1.464599	-0.347992
H	2.988490	1.050564	-1.642210
C	4.175349	1.539287	2.013405
H	2.113985	1.240893	2.556665
C	5.092755	1.622673	0.966318
H	5.379252	1.489848	-1.163374
H	4.509601	1.638022	3.041823
H	6.145086	1.787526	1.177612
C	-1.742421	0.668777	-1.240770
H	-1.104300	-0.207519	-1.058744
O	-1.598371	1.102487	-2.560591
H	-0.831256	0.587452	-2.936130
C	-3.181190	0.268192	-0.945975
C	-3.528348	-0.425421	0.253433
C	-4.186966	0.599746	-1.817527
C	-2.574485	-0.891208	1.191831
C	-4.909030	-0.673861	0.490312
C	-5.528521	0.289073	-1.487863
H	-3.949333	1.095508	-2.752247
C	-2.970623	-1.575294	2.320890
H	-1.512410	-0.764308	1.007459
C	-5.289079	-1.345314	1.684307
H	-6.325490	0.560672	-2.178180
C	-4.351649	-1.781177	2.579398
H	-6.349186	-1.512186	1.848433
H	-4.630764	-2.313609	3.483142
O	-2.097147	-2.090540	3.209494
N	0.114441	2.160117	-0.211321
C	-1.181556	5.105189	1.620515
H	-1.966845	4.471428	2.035463
C	-0.970124	6.310511	2.139717
H	-1.569402	6.687299	2.963135
H	-0.191078	6.966954	1.757972
N	-5.892517	-0.306220	-0.377254
H	-1.199143	-2.109929	2.806680
C	-2.805169	-4.331302	-1.307906
C	-1.864073	-3.595574	-2.022940
C	-0.746133	-3.072963	-1.377360
C	-0.588917	-3.263938	0.000156

	C	-1.536851	-4.006095	0.714610
	C	-2.636211	-4.544657	0.060621
	H	-3.674485	-4.739018	-1.815307
	H	-1.997995	-3.419824	-3.085692
	H	-0.032420	-2.478740	-1.942626
	H	-1.410425	-4.146064	1.783982
	H	-3.369239	-5.119833	0.617725
	C	0.527112	-2.618225	0.745696
	O	0.362558	-2.247261	1.914151
	C	1.821114	-2.447766	0.066284
	H	1.890220	-2.695865	-0.987665
	C	2.897857	-2.060562	0.775282
	H	2.754305	-1.876687	1.840253
	C	4.261032	-1.903238	0.270095
	C	5.309348	-1.794954	1.192514
	C	4.548581	-1.844133	-1.103492
	C	6.624006	-1.654658	0.760294
	H	5.084838	-1.824055	2.256128
	C	5.861929	-1.699709	-1.531038
	H	3.737956	-1.854051	-1.829993
	C	6.901973	-1.609651	-0.603679
	H	7.428549	-1.578048	1.485681
	H	6.076031	-1.647423	-2.594403
	H	7.926773	-1.499179	-0.946452
	C	1.672325	-0.862783	-3.023572
	N	0.657834	-0.270904	-3.064353

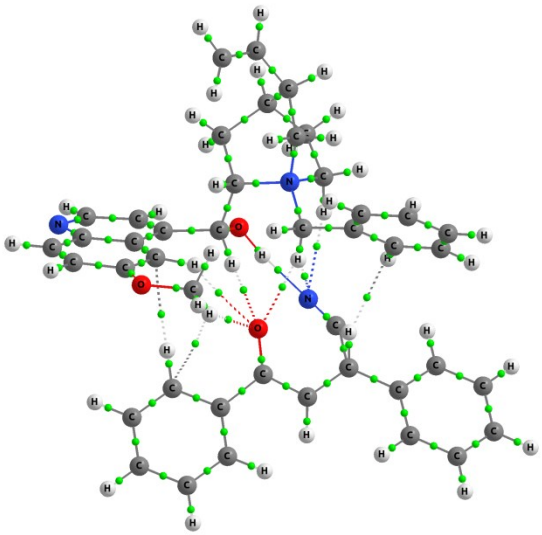
Compound	Coordinates			
	Atom	x	y	z
ts_cat1_R	C	-1.182039	1.828987	-0.579501
Img. freq. = 1	C	-1.757903	4.263314	-0.587012
SCF Energy (a.u.) = -2054.02033832	C	-2.167494	2.881780	-1.102528
	H	-1.514503	1.447293	0.388558
	H	-2.163537	2.877034	-2.198908
	H	-3.174901	2.606777	-0.777733
	C	0.517856	3.541334	-1.309618
	H	1.516564	3.895455	-1.052583
	H	0.554417	2.976073	-2.239240
	C	-0.501893	4.691540	-1.349355
	H	-0.078707	5.598478	-0.905276
	H	-0.745796	4.916353	-2.391229
	H	-2.565175	4.986240	-0.728573
	C	-1.393873	4.185975	0.911157
	H	-1.131516	5.197267	1.242100
	C	-0.124158	3.305618	1.041761



H	0.768054	3.905700	1.231688
H	-0.218379	2.560974	1.837551
C	1.233620	1.514697	-0.025598
H	0.815724	0.793027	0.681909
H	1.392296	1.036606	-0.994647
C	2.536575	2.051768	0.505343
C	3.543005	2.481417	-0.365843
C	2.795653	2.012133	1.879347
C	4.773832	2.903781	0.131010
H	3.370247	2.452555	-1.439468
C	4.026956	2.429591	2.376129
H	2.041791	1.603718	2.549075
C	5.013867	2.883872	1.503183
H	5.549102	3.231682	-0.554786
H	4.222007	2.383823	3.443031
H	5.976094	3.204835	1.890644
C	-1.019825	0.625391	-1.529218
H	-0.418719	-0.149666	-1.029846
O	-0.389004	1.056913	-2.704107
H	0.341348	0.413103	-2.902833
C	-2.394029	0.030526	-1.820730
C	-3.194397	-0.602006	-0.812682
C	-2.898759	0.113629	-3.092121
C	-2.788288	-0.792642	0.529206
C	-4.479530	-1.075692	-1.215544
C	-4.186229	-0.403318	-3.378420
H	-2.307436	0.573507	-3.875020
C	-3.633259	-1.395620	1.441056
H	-1.796023	-0.528306	0.886435
C	-5.314386	-1.697456	-0.257976
H	-4.578133	-0.330292	-4.391686
C	-4.914302	-1.854141	1.044016
H	-6.285857	-2.046051	-0.594106
H	-5.576869	-2.330401	1.757520
O	-3.169031	-1.507488	2.708721
N	0.136216	2.544221	-0.236849
C	-2.532823	3.703326	1.770592
H	-2.837922	2.660962	1.664312
C	-3.180740	4.483118	2.630597
H	-4.009630	4.110240	3.224580
H	-2.904872	5.526229	2.772301
N	-4.960762	-0.968234	-2.488204
C	-2.086221	-4.569496	0.086974
C	-1.350579	-3.920385	-0.899704
C	-0.363613	-3.000570	-0.547263

	C	-0.130491	-2.698963	0.797587
	C	-0.884929	-3.343746	1.783083
	C	-1.838843	-4.291010	1.431709
	H	-2.851843	-5.289010	-0.188978
	H	-1.547191	-4.121571	-1.948648
	H	0.194589	-2.489771	-1.328034
	H	-0.725674	-3.074301	2.822710
	H	-2.402134	-4.805660	2.205625
	C	0.799392	-1.596989	1.238329
	O	0.346978	-0.785206	2.074638
	C	2.132221	-1.488936	0.746386
	H	2.703746	-0.672980	1.180662
	C	2.734844	-2.274025	-0.233674
	H	2.258068	-3.215533	-0.497273
	C	4.222577	-2.293389	-0.332557
	C	4.887694	-3.505635	-0.517727
	C	4.973103	-1.119386	-0.210736
	C	6.279668	-3.550772	-0.562226
	H	4.310587	-4.421118	-0.621679
	C	6.360733	-1.162492	-0.259794
	H	4.461667	-0.166416	-0.093162
	C	7.020089	-2.379989	-0.431836
	H	6.783331	-4.502841	-0.701613
	H	6.929223	-0.241109	-0.167949
	H	8.104929	-2.412860	-0.470294
	C	2.287539	-1.448543	-2.050636
	N	1.673474	-0.684553	-2.690185
	C	-3.901327	-2.300193	3.619298
	H	-3.295034	-2.354413	4.524719
	H	-4.868983	-1.845309	3.865232
	H	-4.064766	-3.312547	3.230760

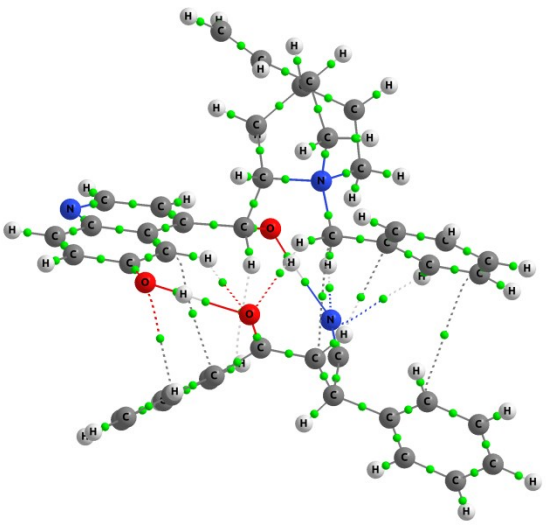
Compound	Coordinates			
	Atom	x	y	z
ts_cat1_S	C	2.038839	-1.598212	-0.424717
Img. freq. = 1	C	2.624683	-3.991039	-0.969829
SCF Energy (a.u.) = -2054.02314160	C	3.123167	-2.548423	-0.978818
	H	2.380188	-1.127812	0.501836
	H	3.357265	-2.260877	-2.006583
	H	4.037169	-2.451467	-0.386718
	C	0.235175	-3.265214	-1.066937
	H	-0.482896	-3.922467	-0.571531
	H	-0.303622	-2.584988	-1.726579
	C	1.333566	-4.058460	-1.788685
	H	1.008870	-5.095502	-1.914628



H	1.504799	-3.625645	-2.776744
H	3.383290	-4.651603	-1.399880
C	2.322525	-4.419169	0.483464
H	1.799513	-5.382283	0.437844
C	1.361393	-3.382540	1.095962
H	0.494288	-3.868584	1.543161
H	1.831842	-2.756712	1.857212
C	-0.204950	-1.509511	0.652253
H	0.338638	-0.883220	1.365865
H	-0.569477	-0.868317	-0.151095
C	-1.361688	-2.203845	1.323703
C	-2.485968	-2.573968	0.577515
C	-1.362523	-2.421408	2.704402
C	-3.582512	-3.165497	1.198190
H	-2.505310	-2.367716	-0.490972
C	-2.456231	-3.017015	3.326220
H	-0.504656	-2.111156	3.297396
C	-3.566127	-3.392353	2.572579
H	-4.455571	-3.432385	0.610620
H	-2.446370	-3.177518	4.399859
H	-4.423153	-3.848646	3.058358
C	1.686257	-0.483902	-1.440541
H	0.850959	0.130558	-1.073978
O	1.363275	-1.056600	-2.677766
H	0.414461	-0.832078	-2.851633
C	2.916806	0.405664	-1.559548
C	3.319754	1.274376	-0.500065
C	3.695974	0.354749	-2.688814
C	2.549441	1.479107	0.679386
C	4.542879	1.980253	-0.668489
C	4.884877	1.116572	-2.754649
H	3.394266	-0.267100	-3.524032
C	2.997597	2.347365	1.651521
H	1.562624	1.034226	0.759494
C	4.985114	2.845544	0.370741
H	5.502977	1.068912	-3.649445
C	4.241214	3.022091	1.500854
H	5.927127	3.364321	0.223060
H	4.559109	3.687246	2.297489
O	2.326852	2.645354	2.785027
N	0.838071	-2.434864	0.045296
C	3.595182	-4.633015	1.264903
H	4.090981	-5.578067	1.044596
C	4.184622	-3.797280	2.115892
H	5.129629	-4.059138	2.582066

	H	3.776588	-2.827286	2.389570
	N	5.315799	1.887771	-1.784869
	C	-0.386496	6.352304	0.515538
	C	0.554502	5.349131	0.287907
	C	0.138855	4.033560	0.116084
	C	-1.218485	3.703768	0.161801
	C	-2.155955	4.715756	0.389124
	C	-1.741693	6.032478	0.568160
	H	-0.064417	7.380465	0.653337
	H	1.612923	5.590072	0.243886
	H	0.860892	3.244165	-0.067328
	H	-3.211772	4.467722	0.450039
	H	-2.477684	6.809603	0.752504
	C	-1.622872	2.263838	0.002767
	O	-0.805607	1.376108	0.325503
	C	-2.924743	1.980681	-0.510094
	H	-3.492199	2.769348	-0.992346
	C	-3.365648	0.668362	-0.561518
	H	-2.840323	-0.016940	0.102786
	C	-4.801981	0.333870	-0.810730
	C	-5.205564	-0.889071	-1.359320
	C	-5.791754	1.232944	-0.399954
	C	-6.553088	-1.202412	-1.492144
	H	-4.448572	-1.579875	-1.716946
	C	-7.143383	0.924267	-0.539496
	H	-5.495833	2.174274	0.052863
	C	-7.530095	-0.295243	-1.084522
	H	-6.843144	-2.153737	-1.929429
	H	-7.892901	1.639974	-0.214273
	H	-8.583031	-0.537439	-1.194987
	C	-2.342507	-0.310294	-2.085492
	N	-1.293966	-0.538231	-2.552441
	C	1.099564	1.971689	3.012380
	H	0.388113	2.126266	2.193976
	H	1.273381	0.893597	3.141959
	H	0.699218	2.383204	3.939441

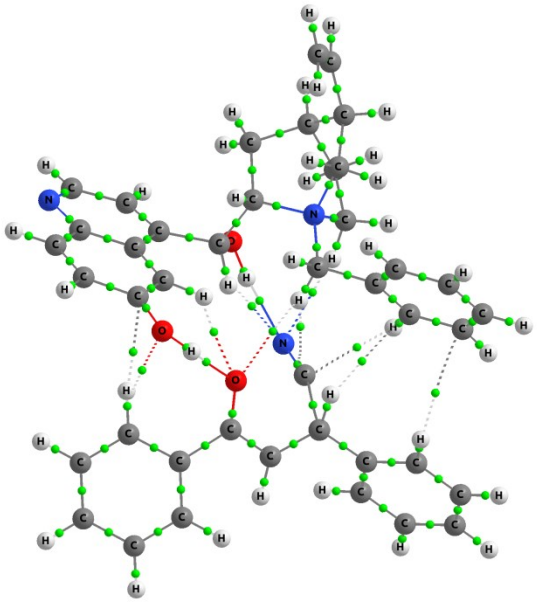
Compound	Coordinates			
	Atom	x	y	z
ts_cat2_R	C	-1.613756	1.752598	-0.464939
Img. freq. = 1	C	-2.066358	4.205355	-0.760910
SCF Energy (a.u.) = -2014.74860115	C	-2.559705	2.794036	-1.084454
	H	-1.986735	1.434657	0.514317
	H	-2.579101	2.660138	-2.170522
	H	-3.565768	2.612052	-0.703371



C	0.202235	3.274481	-1.294816
H	1.195452	3.633730	-1.024883
H	0.280234	2.591422	-2.139225
C	-0.775459	4.435906	-1.554525
H	-0.318717	5.388175	-1.266981
H	-0.996429	4.483156	-2.623921
H	-2.815346	4.950571	-1.041824
C	-1.732366	4.325250	0.734615
H	-1.369763	5.345522	0.916769
C	-0.546779	3.375487	1.031209
H	0.383515	3.920852	1.197878
H	-0.738914	2.740101	1.900658
C	0.756070	1.411036	0.279455
H	0.291968	0.811965	1.071806
H	0.924944	0.787677	-0.598457
C	2.079399	1.973747	0.733856
C	3.119906	2.113581	-0.190507
C	2.321774	2.257853	2.081819
C	4.368302	2.576751	0.218327
H	2.955589	1.824204	-1.226424
C	3.571210	2.714634	2.491669
H	1.535885	2.094848	2.815674
C	4.592921	2.884394	1.558049
H	5.170520	2.670805	-0.506880
H	3.750524	2.926270	3.541193
H	5.568428	3.236815	1.879432
C	-1.489914	0.507051	-1.377219
H	-0.754305	-0.196596	-0.967027
O	-1.119385	0.890479	-2.674913
H	-0.250524	0.464719	-2.866606
C	-2.841160	-0.191449	-1.367047
C	-3.262081	-0.937329	-0.225192
C	-3.688097	-0.109199	-2.442179
C	-2.446061	-1.138198	0.912541
C	-4.557816	-1.522866	-0.265737
C	-4.958039	-0.732402	-2.374526
H	-3.381087	0.420774	-3.337118
C	-2.882714	-1.904581	1.972991
H	-1.444691	-0.727296	0.960210
C	-4.997926	-2.277994	0.856496
H	-5.634231	-0.660246	-3.224652
C	-4.189489	-2.466663	1.943611
H	-5.992274	-2.711246	0.809526
H	-4.511858	-3.057518	2.795225
O	-2.120969	-2.149497	3.050581

	N	-0.281957	2.445749	-0.126634
	C	-2.889323	4.086492	1.676520
	H	-2.608757	3.849860	2.703543
	C	-4.180182	4.187747	1.373532
	H	-4.944585	4.032950	2.128646
	H	-4.529057	4.433700	0.373887
	N	-5.393435	-1.404097	-1.334667
	H	-1.182800	-1.883468	2.849420
	C	-1.317669	-5.182873	-0.357233
	C	-0.829192	-4.191105	-1.203019
	C	-0.059748	-3.149677	-0.688754
	C	0.211585	-3.086239	0.681494
	C	-0.289053	-4.082380	1.526224
	C	-1.039824	-5.131117	1.008156
	H	-1.917724	-5.993703	-0.759355
	H	-1.052751	-4.219998	-2.265089
	H	0.304695	-2.372293	-1.355340
	H	-0.092327	-4.022388	2.592322
	H	-1.419711	-5.902655	1.671041
	C	0.918132	-1.915360	1.304375
	O	0.396606	-1.409772	2.333590
	C	2.130150	-1.393894	0.782962
	H	2.507102	-0.535943	1.328654
	C	2.837231	-1.874034	-0.318396
	H	2.529285	-2.835422	-0.723071
	C	4.296496	-1.595056	-0.488708
	C	4.977015	-2.181815	-1.562134
	C	5.014543	-0.800009	0.406234
	C	6.339673	-1.983424	-1.737758
	H	4.415905	-2.785112	-2.271942
	C	6.381168	-0.590507	0.225869
	H	4.517225	-0.343976	1.256415
	C	7.048149	-1.181312	-0.842095
	H	6.850604	-2.449668	-2.574769
	H	6.922868	0.033998	0.930592
	H	8.113711	-1.021655	-0.977635
	C	2.142850	-0.921245	-2.018319
	N	1.395737	-0.226433	-2.592331

Compound	Coordinates			
	Atom	x	y	z
ts_cat2_S	C	2.683549	-0.600712	-0.410250
Img. freq. = 1	C	4.131091	-2.570045	-1.048589
SCF Energy (a.u.) = -2014.74394074	C	4.074136	-1.047008	-0.918313
	H	2.777359	-0.025106	0.514764



H	4.256298	-0.593684	-1.894883
H	4.851079	-0.695379	-0.232892
C	1.645221	-2.784347	-1.119249
H	1.249004	-3.697567	-0.670770
H	0.867523	-2.326194	-1.732364
C	2.947026	-3.042549	-1.894223
H	3.031566	-4.112134	-2.107056
H	2.925728	-2.497741	-2.839229
H	5.075401	-2.870128	-1.512151
C	4.008798	-3.197572	0.351814
H	3.806792	-4.268879	0.212214
C	2.793766	-2.558718	1.043492
H	2.180111	-3.304240	1.548174
H	3.082081	-1.790273	1.765309
C	0.610935	-1.432008	0.722264
H	0.905200	-0.718313	1.496787
H	0.013461	-0.913198	-0.028833
C	-0.181811	-2.567900	1.318419
C	-1.073571	-3.305914	0.531992
C	-0.070799	-2.865307	2.680654
C	-1.807056	-4.349265	1.092316
H	-1.211199	-3.046362	-0.515960
C	-0.810008	-3.901806	3.242466
H	0.592561	-2.271995	3.305960
C	-1.672800	-4.651493	2.445579
H	-2.498760	-4.909956	0.471103
H	-0.717418	-4.118698	4.302007
H	-2.250064	-5.460662	2.882311
C	1.951932	0.290701	-1.447061
H	0.903376	0.428401	-1.166463
O	2.010129	-0.269137	-2.731165
H	1.073495	-0.423232	-2.991945
C	2.638628	1.645978	-1.387191
C	2.351980	2.539655	-0.312188
C	3.574379	2.024812	-2.314176
C	1.331930	2.294166	0.636204
C	3.114714	3.735542	-0.224963
C	4.263587	3.251776	-2.142567
H	3.783026	1.392900	-3.171091
C	1.060360	3.206641	1.634008
H	0.685893	1.428891	0.553077
C	2.853801	4.629705	0.850365
H	5.014960	3.547448	-2.872628
C	1.859164	4.377220	1.757049
H	3.455389	5.531652	0.908697

	H	1.634368	5.071144	2.560900
	O	0.037004	3.042476	2.491098
	N	1.909148	-1.850322	0.040659
	C	5.290334	-3.089875	1.137189
	H	6.159304	-3.474296	0.602460
	C	5.464305	-2.615372	2.367505
	H	6.451171	-2.606232	2.819790
	H	4.656476	-2.233107	2.985099
	N	4.071007	4.071254	-1.135904
	H	-0.604437	2.406819	2.077125
	C	-3.687989	5.846792	0.591452
	C	-2.356837	5.480729	0.401128
	C	-2.004249	4.136213	0.356027
	C	-2.981357	3.145404	0.482327
	C	-4.317267	3.518218	0.657445
	C	-4.667225	4.863812	0.721568
	H	-3.962608	6.896621	0.634962
	H	-1.591224	6.242453	0.287566
	H	-0.972040	3.845137	0.186886
	H	-5.078200	2.750156	0.764547
	H	-5.704930	5.145547	0.873250
	C	-2.573209	1.702926	0.424352
	O	-1.508816	1.348247	0.988428
	C	-3.417472	0.809841	-0.290991
	H	-4.250162	1.208287	-0.860022
	C	-3.116522	-0.542340	-0.345763
	H	-2.418452	-0.904962	0.406621
	C	-4.140691	-1.522432	-0.793355
	C	-4.735639	-1.435030	-2.055189
	C	-4.560019	-2.518942	0.090592
	C	-5.736135	-2.327117	-2.423646
	H	-4.387670	-0.675384	-2.750535
	C	-5.565458	-3.411512	-0.277592
	H	-4.103698	-2.585785	1.074894
	C	-6.154762	-3.317968	-1.535054
	H	-6.186669	-2.255087	-3.409063
	H	-5.887533	-4.178908	0.420459
	H	-6.934941	-4.015221	-1.825314
	C	-1.643271	-0.882490	-1.843004
	N	-0.727455	-0.745199	-2.558713

Compound	Coordinates			
	Atom	x	y	z
prod_cat1_S	C	1.990619	-1.441513	-0.493719
Img. freq. = 0	C	2.638954	-3.750910	-1.308927

SCF Energy (a.u.) = -2054.05474070	C	3.075518	-2.288734	-1.199737
	H	2.382346	-1.003720	0.428559
	H	3.231859	-1.896185	-2.207081
	H	4.025295	-2.195522	-0.665495
	C	0.225191	-3.144110	-1.110326
	H	-0.398297	-3.895029	-0.621335
	H	-0.419524	-2.441453	-1.636583
	C	1.283619	-3.785581	-2.020356
	H	0.990875	-4.815585	-2.243095
	H	1.345203	-3.229783	-2.957936
	H	3.382810	-4.322768	-1.870053
	C	2.462542	-4.361379	0.093989
	H	1.940763	-5.319724	-0.014644
	C	1.572974	-3.398375	0.909401
	H	0.789122	-3.936353	1.443027
	H	2.153959	-2.820714	1.635088
	C	-0.121776	-1.592269	0.821407
	H	0.461858	-1.075481	1.589980
	H	-0.541155	-0.821739	0.172127
	C	-1.218224	-2.410102	1.455928
	C	-2.372307	-2.737161	0.734616
	C	-1.133547	-2.787947	2.799133
	C	-3.408748	-3.443689	1.338165
	H	-2.461371	-2.427901	-0.304756
	C	-2.168954	-3.494182	3.405739
	H	-0.253693	-2.514441	3.377034
	C	-3.307057	-3.825231	2.674624
	H	-4.300215	-3.682875	0.766584
	H	-2.090222	-3.776241	4.451008
	H	-4.117979	-4.370146	3.147944
	C	1.490553	-0.277372	-1.388834
	H	0.655440	0.258493	-0.915302
	O	1.111330	-0.779118	-2.650719
	H	0.164693	-0.578417	-2.779947
	C	2.673112	0.675650	-1.525077
	C	3.117534	1.473627	-0.424138
	C	3.400265	0.715415	-2.688489
	C	2.378462	1.615410	0.782590
	C	4.358544	2.154256	-0.574306
	C	4.591873	1.476892	-2.743896
	H	3.070285	0.150077	-3.552796
	C	2.893260	2.365093	1.817499
	H	1.363786	1.225985	0.832879
	C	4.872129	2.889348	0.528181
	H	5.168010	1.501272	-3.667310

C	4.168967	2.979894	1.696724
H	5.828303	3.386782	0.399268
H	4.540215	3.551276	2.541529
O	2.269489	2.555522	3.008747
N	0.891662	-2.387911	0.015391
C	3.760554	-4.614564	0.808009
H	4.380506	-3.740076	1.010150
C	4.176702	-5.817528	1.191172
H	5.128848	-5.956966	1.693961
H	3.579953	-6.709292	1.012047
N	5.083230	2.145328	-1.728284
C	-0.102146	6.168564	0.673681
C	0.654293	5.212639	-0.005731
C	0.148693	3.930726	-0.192359
C	-1.120254	3.584066	0.282726
C	-1.874895	4.550272	0.952689
C	-1.367980	5.834196	1.150267
H	0.294245	7.167391	0.832082
H	1.642730	5.463582	-0.381137
H	0.735763	3.174989	-0.705116
H	-2.853542	4.280597	1.340988
H	-1.959169	6.572187	1.685508
C	-1.598569	2.171122	0.105655
O	-0.742614	1.226848	0.307010
C	-2.891160	1.946159	-0.281832
H	-3.588310	2.731780	-0.544376
C	-3.297399	0.505505	-0.481375
H	-3.051472	-0.077288	0.419946
C	-4.764307	0.312471	-0.812399
C	-5.262992	0.637724	-2.075848
C	-5.642433	-0.146565	0.169232
C	-6.619622	0.500257	-2.353700
H	-4.581926	0.998592	-2.843281
C	-7.001345	-0.281496	-0.106873
H	-5.257338	-0.394751	1.155281
C	-7.492573	0.040182	-1.369354
H	-6.996071	0.753703	-3.340235
H	-7.675798	-0.638748	0.665754
H	-8.551149	-0.066384	-1.586319
C	-2.436772	-0.086470	-1.534224
N	-1.721934	-0.532880	-2.329845
C	0.851631	2.712550	2.995716
H	0.337916	1.940388	2.414102
H	0.537972	2.656906	4.039829
H	0.590570	3.694750	2.587105

Compound	Coordinates			
	Atom	x	y	z
prod_cat1_R	C	-1.251324	1.714418	-0.738918
Img. freq. = 0	C	-2.302594	3.972251	-0.907727
SCF Energy (a.u.) = -2054.04736209	C	-2.397429	2.514780	-1.369450
	H	-1.548765	1.345072	0.243511
	H	-2.336131	2.462159	-2.463008
	H	-3.343804	2.054035	-1.073093
	C	0.096403	3.691757	-1.517807
	H	0.995509	4.249231	-1.255362
	H	0.279878	3.102934	-2.415037
	C	-1.126273	4.615878	-1.645876
	H	-0.909270	5.604016	-1.227406
	H	-1.365371	4.749417	-2.704414
	H	-3.233360	4.506803	-1.112807
	C	-1.996982	4.029495	0.605441
	H	-1.966760	5.084809	0.898853
	C	-0.577172	3.443314	0.822404
	H	0.161282	4.226773	1.000933
	H	-0.540458	2.733992	1.654473
	C	1.158299	1.913628	-0.112168
	H	0.843809	1.095416	0.547868
	H	1.487778	1.526797	-1.078603
	C	2.240602	2.698838	0.580723
	C	3.148196	3.506602	-0.112101
	C	2.381900	2.544530	1.964773
	C	4.144831	4.195096	0.574485
	H	3.092712	3.577596	-1.195790
	C	3.379549	3.232245	2.650069
	H	1.728004	1.840920	2.477092
	C	4.253651	4.067610	1.957646
	H	4.845916	4.818120	0.027644
	H	3.484507	3.102779	3.722878
	H	5.034636	4.600744	2.491421
	C	-0.820495	0.486105	-1.558854
	H	-0.141027	-0.127541	-0.948287
	O	-0.163799	0.936409	-2.722117
	H	0.462990	0.237443	-3.000543
	C	-2.056502	-0.345633	-1.891668
	C	-2.853371	-0.983208	-0.882590
	C	-2.444353	-0.469847	-3.200307
	C	-2.557055	-0.962329	0.501820
	C	-4.010570	-1.689201	-1.330354
	C	-3.608530	-1.208459	-3.527378

	H	-1.864827	0.002258	-3.984707
	C	-3.392205	-1.590955	1.405234
	H	-1.640626	-0.531824	0.903627
	C	-4.836545	-2.330106	-0.376867
	H	-3.906037	-1.301954	-4.570518
	C	-4.547598	-2.283578	0.962247
	H	-5.709189	-2.859010	-0.746808
	H	-5.199205	-2.780173	1.671836
	O	-3.047771	-1.493131	2.711635
	N	-0.116691	2.693102	-0.405681
	C	-3.048723	3.350618	1.444158
	H	-3.121647	2.263797	1.379941
	C	-3.886991	4.008835	2.238822
	H	-4.644844	3.491371	2.818944
	H	-3.844454	5.091494	2.339327
	N	-4.374446	-1.791963	-2.642226
	C	-1.544635	-4.720058	0.984624
	C	-1.075225	-4.175910	-0.207150
	C	-0.217798	-3.076163	-0.183423
	C	0.164811	-2.490037	1.027658
	C	-0.336147	-3.031141	2.216736
	C	-1.161302	-4.149506	2.199588
	H	-2.208486	-5.579790	0.968325
	H	-1.386182	-4.596124	-1.159398
	H	0.106493	-2.641009	-1.126731
	H	-0.081541	-2.542860	3.152454
	H	-1.520444	-4.570933	3.135155
	C	0.983383	-1.219498	1.130128
	O	0.470255	-0.303693	1.868779
	C	2.189017	-1.096685	0.470728
	H	2.750503	-0.174680	0.607237
	C	2.758616	-2.049737	-0.548745
	H	2.307224	-3.043882	-0.427231
	C	4.277035	-2.208227	-0.508276
	C	4.912569	-2.251824	0.733926
	C	5.040968	-2.353632	-1.666766
	C	6.288110	-2.445201	0.815429
	H	4.314818	-2.125568	1.632025
	C	6.419175	-2.541260	-1.585714
	H	4.560676	-2.316476	-2.641711
	C	7.047080	-2.588975	-0.344462
	H	6.769292	-2.478572	1.788533
	H	7.001050	-2.647999	-2.496495
	H	8.121333	-2.734144	-0.280774
	C	2.297478	-1.561161	-1.870092

	N	1.832861	-1.104908	-2.830066
	C	-3.732777	-2.307750	3.638846
	H	-3.205459	-2.193495	4.587170
	H	-4.773843	-1.985950	3.768166
	H	-3.712706	-3.361817	3.337982

Compound	Coordinates			
	Atom	x	y	z
prod_cat2_R	C	-2.041648	-1.312464	0.671768
Img. freq. = 0	C	-3.422655	-3.388403	0.870630
SCF Energy (a.u.) = -2014.78073121	C	-3.306425	-1.922191	1.294522
	H	-2.274919	-0.867967	-0.298605
	H	-3.250087	-1.853533	2.386342
	H	-4.170668	-1.336940	0.970902
	C	-0.990348	-3.460209	1.430916
	H	-0.197913	-4.155617	1.155416
	H	-0.696008	-2.892765	2.313302
	C	-2.339347	-4.177701	1.609910
	H	-2.284456	-5.200177	1.223029
	H	-2.572487	-4.237967	2.676296
	H	-4.415828	-3.780232	1.103182
	C	-3.158431	-3.522364	-0.643880
	H	-3.280082	-4.577326	-0.913591
	C	-1.677588	-3.142182	-0.899893
	H	-1.060253	-4.021751	-1.089013
	H	-1.565392	-2.453849	-1.742634
	C	0.291938	-1.885920	-0.020997
	H	0.119614	-1.006735	-0.651891
	H	0.711471	-1.566969	0.937022
	C	1.219443	-2.827778	-0.743453
	C	1.996080	-3.770440	-0.062536
	C	1.361405	-2.696984	-2.129141
	C	2.854872	-4.612186	-0.764008
	H	1.951996	-3.828781	1.022215
	C	2.222304	-3.537049	-2.828934
	H	0.834457	-1.894281	-2.640520
	C	2.958738	-4.504757	-2.148917
	H	3.455381	-5.339443	-0.226618
	H	2.330854	-3.422987	-3.902854
	H	3.633614	-5.157320	-2.694286
	C	-1.427032	-0.204174	1.543936
	H	-0.507039	0.167041	1.073236
	O	-1.141299	-0.726419	2.819585
	H	-0.323504	-0.292162	3.131924
	C	-2.418547	0.948531	1.573473

	C	-2.599602	1.748710	0.404967
	C	-3.163375	1.235855	2.687590
	C	-1.850535	1.563412	-0.776709
	C	-3.563731	2.792235	0.465887
	C	-4.098109	2.300287	2.637087
	H	-3.033512	0.658909	3.597182
	C	-2.014571	2.391287	-1.871799
	H	-1.076250	0.810594	-0.840898
	C	-3.747652	3.608201	-0.685523
	H	-4.694766	2.528491	3.518552
	C	-3.001947	3.418510	-1.817752
	H	-4.490416	4.397940	-0.625062
	H	-3.124269	4.055518	-2.688252
	O	-1.274082	2.267892	-2.972872
	N	-1.081500	-2.454880	0.306588
	C	-4.117481	-2.717727	-1.480887
	H	-4.038816	-1.631144	-1.426444
	C	-5.045120	-3.262348	-2.261880
	H	-5.730123	-2.651315	-2.841495
	H	-5.152722	-4.341401	-2.350635
	N	-4.306211	3.048499	1.578566
	H	-0.455206	1.688168	-2.755109
	C	0.569217	5.545058	-0.643725
	C	0.432428	4.667895	0.428700
	C	0.717857	3.314426	0.262364
	C	1.138488	2.818469	-0.976090
	C	1.252965	3.707021	-2.049907
	C	0.982304	5.060965	-1.884167
	H	0.344910	6.600104	-0.516964
	H	0.089084	5.032161	1.392473
	H	0.571574	2.630684	1.096770
	H	1.544314	3.318732	-3.021680
	H	1.081658	5.738980	-2.726902
	C	1.387300	1.351351	-1.226636
	O	0.758202	0.827419	-2.233274
	C	2.247030	0.639015	-0.430062
	H	2.429912	-0.401696	-0.685953
	C	2.980282	1.149465	0.786044
	H	2.956888	2.247392	0.800160
	C	4.437905	0.700233	0.886414
	C	5.208060	0.667705	-0.277707
	C	5.032239	0.365554	2.103522
	C	6.551975	0.311517	-0.223342
	H	4.740263	0.918998	-1.225279
	C	6.376730	0.003474	2.156995

	H	4.445054	0.383078	3.018503
	C	7.140989	-0.023753	0.994274
	H	7.139644	0.291989	-1.136371
	H	6.824655	-0.258143	3.111090
	H	8.188535	-0.306536	1.035558
	C	2.201992	0.720643	1.970625
	N	1.500265	0.362094	2.820605

Compound	Coordinates			
	Atom	x	y	z
prod_cat2_S	C	2.595013	-0.801940	-0.233086
Img. freq. = 0	C	4.309640	-2.523138	0.392848
SCF Energy (a.u.) = -2014.78010962	C	4.063088	-1.229945	-0.389943
	H	2.477948	-0.111211	0.608853
	H	4.285972	-1.393519	-1.450017
	H	4.705028	-0.417826	-0.040976
	C	2.143496	-3.244589	-0.619008
	H	1.429761	-4.023322	-0.346528
	H	1.987775	-2.948521	-1.655952
	C	3.596064	-3.664587	-0.337481
	H	3.621999	-4.575978	0.267975
	H	4.095115	-3.881283	-1.285606
	H	5.380699	-2.724405	0.472027
	C	3.701979	-2.413091	1.806622
	H	3.916872	-3.347315	2.336984
	C	2.164230	-2.305213	1.648030
	H	1.659935	-3.232042	1.926778
	H	1.745499	-1.488463	2.242762
	C	0.309814	-1.725996	0.092953
	H	0.170634	-0.735477	0.542849
	H	0.127901	-1.662849	-0.981000
	C	-0.640132	-2.716759	0.711922
	C	-1.185866	-3.743808	-0.065413
	C	-1.087269	-2.542220	2.025038
	C	-2.135656	-4.607849	0.471553
	H	-0.889403	-3.843734	-1.107479
	C	-2.030147	-3.410881	2.566321
	H	-0.718281	-1.706206	2.614256
	C	-2.547976	-4.447320	1.792762
	H	-2.566787	-5.389079	-0.146002
	H	-2.374827	-3.265672	3.585199
	H	-3.295636	-5.114370	2.211110
	C	2.041713	-0.075135	-1.472893
	H	0.992966	0.180318	-1.312218
	O	2.149378	-0.910631	-2.602974

H	1.389029	-0.697844	-3.176590
C	2.804393	1.230362	-1.596454
C	2.453795	2.317983	-0.741106
C	3.854383	1.380966	-2.464874
C	1.342383	2.289939	0.133029
C	3.278953	3.476406	-0.795397
C	4.588261	2.592332	-2.454223
H	4.121371	0.581258	-3.148336
C	1.047672	3.371206	0.944401
H	0.645271	1.458850	0.154849
C	2.976652	4.562190	0.073590
H	5.425584	2.717204	-3.138416
C	1.904809	4.512490	0.921211
H	3.621110	5.434887	0.027433
H	1.660262	5.344987	1.573615
O	-0.007473	3.391768	1.754303
N	1.786896	-2.032778	0.211971
C	4.280402	-1.280600	2.612634
H	4.056568	-0.266064	2.280493
C	5.044502	-1.459598	3.685607
H	5.457561	-0.620050	4.236115
H	5.284881	-2.455208	4.052865
N	4.336047	3.595037	-1.644949
H	-0.629784	2.605943	1.522197
C	-4.257564	5.624455	1.162935
C	-4.199900	5.200030	-0.162935
C	-3.612029	3.979566	-0.482339
C	-3.073752	3.162957	0.517719
C	-3.121335	3.607127	1.842770
C	-3.713522	4.823676	2.165232
H	-4.714432	6.577864	1.412000
H	-4.604478	5.826363	-0.953007
H	-3.545750	3.664887	-1.519739
H	-2.687042	2.981011	2.616409
H	-3.747849	5.150075	3.200817
C	-2.455102	1.825385	0.219324
O	-1.492985	1.426575	1.001188
C	-2.977549	1.089207	-0.809037
H	-3.824495	1.429642	-1.391139
C	-2.426586	-0.285122	-1.069377
H	-1.785577	-0.477228	-0.197749
C	-3.448341	-1.412963	-1.132179
C	-3.614163	-2.242624	-2.239716
C	-4.223471	-1.637334	0.009895
C	-4.540812	-3.285670	-2.207138

	H	-3.019936	-2.079578	-3.135528
	C	-5.143308	-2.677948	0.043540
	H	-4.094396	-0.984002	0.869455
	C	-5.304331	-3.508823	-1.066424
	H	-4.664925	-3.920208	-3.079929
	H	-5.734232	-2.845208	0.939501
	H	-6.025634	-4.320300	-1.041557
	C	-1.501320	-0.319004	-2.220924
	N	-0.707844	-0.361224	-3.065142