CIF-reports for compounds

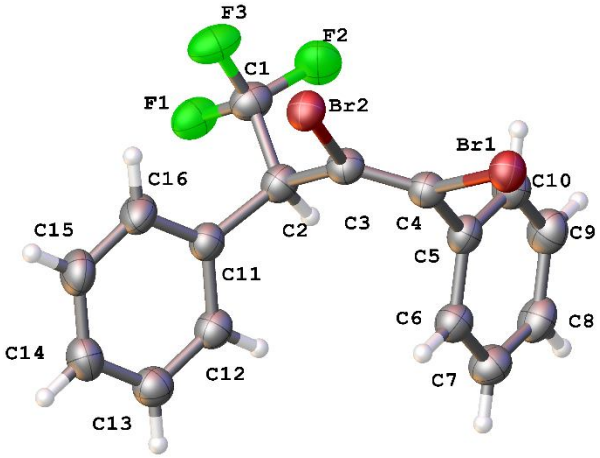


Table S1 Crystal data and structure refinement for *Z*-5a

Empirical formula	2 ($C_{16}H_{11}Br_2F_3$)
Formula weight	840.13
Temperature/K	100 (2)
Crystal system	triclinic
Space group	P-1
a/Å	7.1399(2)
b/Å	9.7404(3)
c/Å	22.8361(6)
α/°	97.673(2)
β/°	97.146(2)
γ/°	106.455(3)
Volume/$Å^3$	1487.30(8)
Z	2
$\rho_{calc}mg/mm^3$	1.876
m/mm^{-1}	7.138
F(000)	816.0
Crystal size/mm^3	0.18× 0.16 × 0.14
Index ranges	$-8 \le h \le 8$, $-11 \le k \le 11$, $-27 \le l \le 27$
Reflections collected	33518
Independent reflections	5637[R(int) = 0.0832]
Data/restraints/parameters	5637/0/379
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0469, wR_2 = 0.1234
Final R indexes [all data]	R_1 = 0.0498, wR_2 = 0.1276
Largest diff. peak/hole / e $Å^{-3}$	1.04/-0.79

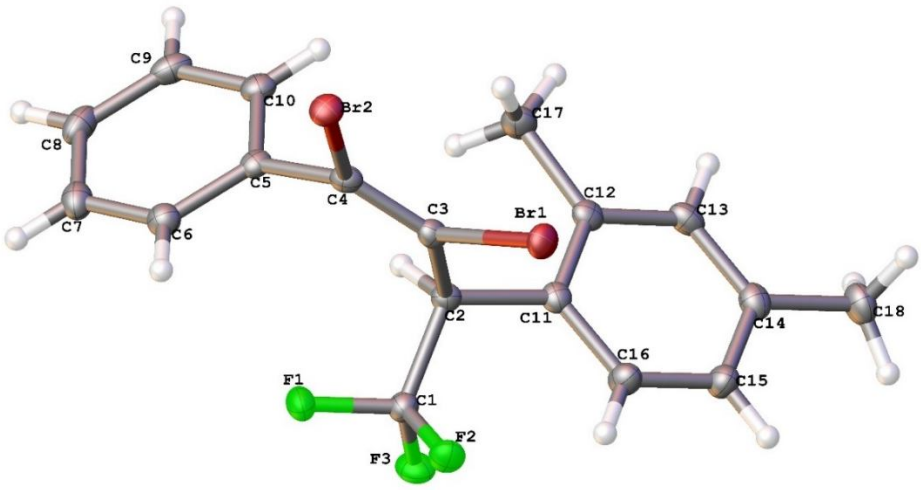


Table S2 Crystal data and structure refinement for *Z*-5c

Empirical formula	$C_{18}H_{15}Br_2F_3$
Formula weight	448.12
Temperature/K	100.01(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	16.4974(2)
b/Å	6.84171(10)
c/Å	28.6498(3)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	3233.71(7)
Z	8
ρ_{calc}mg/mm^3	1.841
m/mm^{-1}	6.611
F(000)	1760.0
Crystal size/mm^3	0.32 × 0.22 × 0.08
2Θ range for data collection	6.16 to 144.98°
Index ranges	$-20 \le h \le 20$, $-8 \le k \le 7$, $-35 \le l \le 35$
Reflections collected	38981
Independent reflections	3212[R(int) = 0.0577]
Data/restraints/parameters	3212/0/210
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0232, wR_2 = 0.0596
Final R indexes [all data]	R_1 = 0.0263, wR_2 = 0.0612
Largest diff. peak/hole / e Å^{-3}	0.59/-0.42

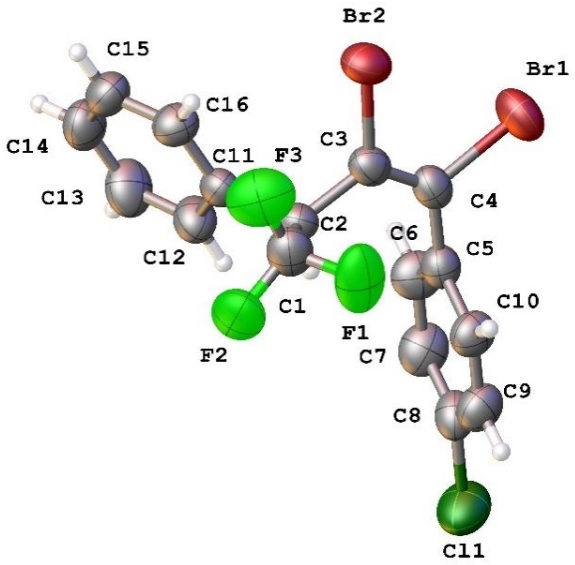


Table S3 Crystal data and structure refinement for *Z*-5i

Empirical formula	$C_{16}H_{10}Br_2ClF_3$
Formula weight	454.49
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	7.3184(2)
b/Å	13.4865(3)
c/Å	17.4149(4)
α/°	101.672(2)
β/°	94.139(2)
γ/°	101.918(2)
Volume/Å^3	1635.33(7)
Z	2
ρ_{calc}mg/mm^3	1.846
m/mm^{-1}	8.018
F(000)	880
Crystal size/mm^3	0.14 × 0.11 × 0.07
2Θ range for data collection	6.88 to 141.98°
Index ranges	$-8 \le h \le 8$, $-16 \le k \le 16$, $-21 \le l \le 21$
Reflections collected	33701
Independent reflections	6300 [R_{int} = 0.0826, R_{sigma} = 0.0433]
Data/restraints/parameters	6300/0/397
Goodness-of-fit on F^2	1.067
Final R indexes [I>=2σ (I)]	R_1 = 0.0454, wR_2 = 0.1445
Final R indexes [all data]	R_1 = 0.0611, wR_2 = 0.1869
Largest diff. peak/hole / e Å^{-3}	0.92/-1.20

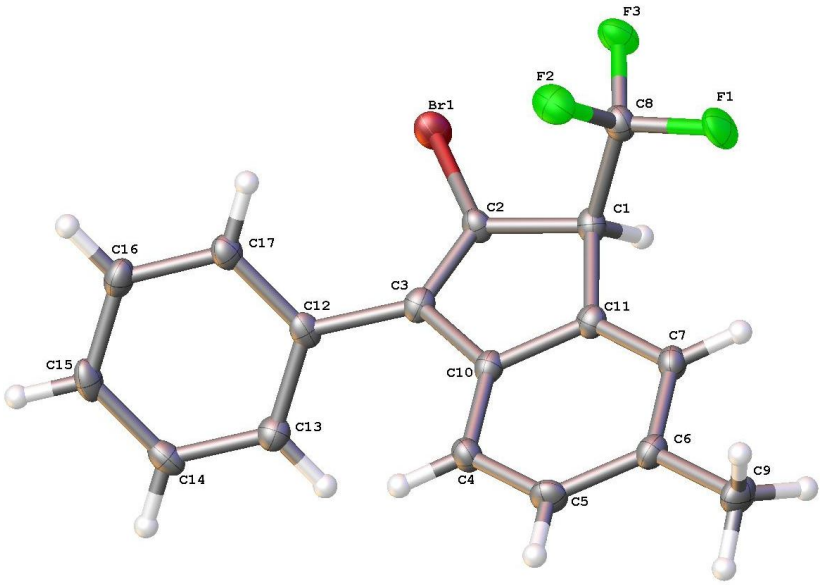


Table S4 Crystal data and structure refinement for 6d

Empirical formula	$C_{17}H_{12}BrF_3$
Formula weight	353.18
Temperature/K	100(2)
Crystal system	monoclinic
Space group	C12/c1
a/Å	22.8229(15)
b/Å	7.4881(4)
c/Å	16.5828(11)
α/°	90.00
β/°	102.102(7)
γ/°	90.00
Volume/Å^3	2771.0(3)
Z	8
ρ_{calc}mg/mm^3	1.693
m/mm^{-1}	4.282
F(000)	1408.0
Crystal size/mm^3	0.23 × 0.17 × 0.09
Index ranges	$-26 \leq h \leq 28$, $-9 \leq k \leq 8$, $-18 \leq l \leq 20$
Reflections collected	7552
Independent reflections	2738[R(int) = 0.0443]
Data/restraints/parameters	2738/0/191
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0379, wR_2 = 0.0933
Final R indexes [all data]	R_1 = 0.0498, wR_2 = 0.1027
Largest diff. peak/hole / e Å^{-3}	0.63/-0.38

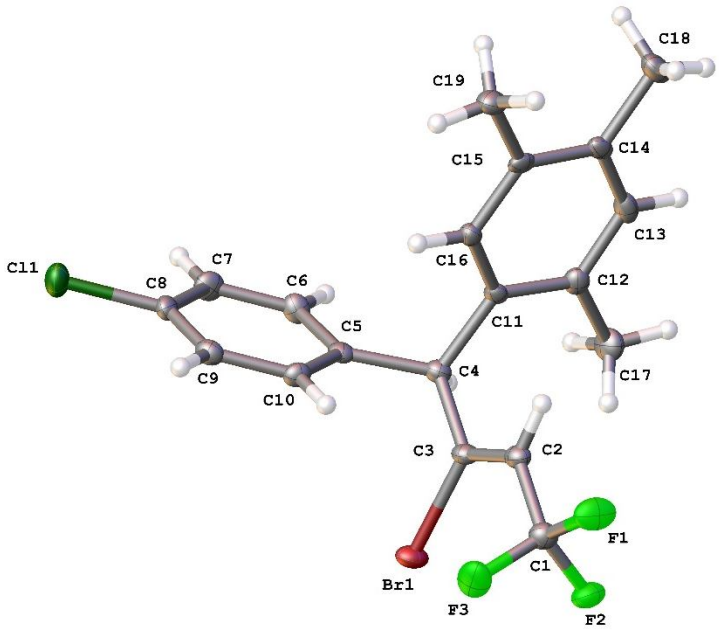


Table S5 Crystal data and structure refinement for 8o

Empirical formula	$C_{19}H_{17}BrClF_3$
Formula weight	417.69
Temperature/K	100(2)
Crystal system	monoclinic
Space group	P121/c1
a/Å	8.2233(3)
b/Å	22.8182(7)
c/Å	10.0565(3)
α/°	90.00
β/°	109.447(4)
γ/°	90.00
Volume/Å^3	1779.35(11)
Z	4
ρ_{calc}mg/mm^3	1.559
m/mm^{-1}	2.487
F(000)	840.0
Crystal size/mm^3	0.15 × 0.10 × 0.08
Index ranges	$-10 \le h \le 10$, $-29 \le k \le 28$, $-13 \le l \le 12$
Reflections collected	10596
Independent reflections	3970[R(int) = 0.0237]
Data/restraints/parameters	3970/0/220
Goodness-of-fit on F^2	1.011
Final R indexes [I>=2σ (I)]	R_1 = 0.0266, wR_2 = 0.0598
Final R indexes [all data]	R_1 = 0.0347, wR_2 = 0.0631
Largest diff. peak/hole / e Å^{-3}	0.35/-0.25

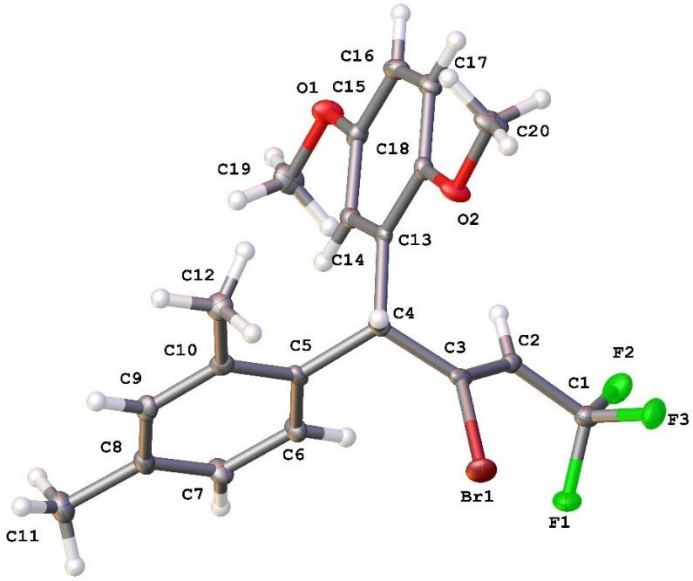


Table S6 Crystal data and structure refinement for 8u

Empirical formula	$C_{20}H_{20}BrF_3O_2$
Formula weight	429.27
Temperature/K	100(2)
Crystal system	triclinic
Space group	P−1
a/Å	8.3533(5)
b/Å	9.4941(4)
c/Å	12.1934(7)
α/°	100.216(4)
β/°	97.306(5)
γ/°	100.289(4)
Volume/Å^3	923.70(8)
Z	2
ρ_{calc}mg/mm^3	1.543
m/mm^{-1}	2.265
F(000)	436
Crystal size/mm^3	0.16 × 0.12 × 0.08
2Θ range for data collection	5.98 to 54.98°
Index ranges	$-8 \le h \le 10$, $-12 \le k \le 12$, $-15 \le l \le 15$
Reflections collected	10460
Independent reflections	4114 [R_{int} = 0.0270, R_{sigma} = 0.0378]
Data/restraints/parameters	4114/0/239
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0286, wR_2 = 0.0627
Final R indexes [all data]	R_1 = 0.0345, wR_2 = 0.0651
Largest diff. peak/hole / e Å^{-3}	0.41/-0.32

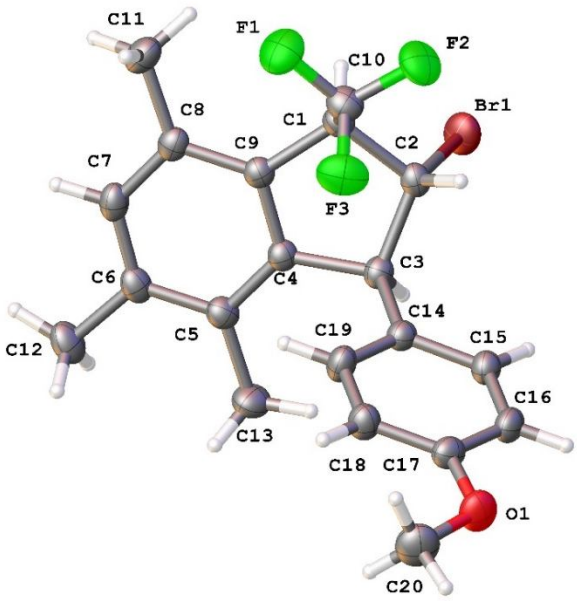


Table S7 Crystal data and structure refinement for 10b

Empirical formula	$C_{20}H_{20}BrF_3O$
Formula weight	413.27
Temperature/K	100(2)
Crystal system	triclinic
Space group	P−1
a/Å	7.8481(5)
b/Å	10.5581(7)
c/Å	12.2042(10)
α/°	75.472(6)
β/°	72.741(6)
γ/°	72.301(6)
Volume/Å^3	905.55(11)
Z	2
ρ_{calc}mg/mm^3	1.516
m/mm^{-1}	3.403
F(000)	420
Crystal size/mm^3	0.14 × 0.10 × 0.04
2Θ range for data collection	7.7 to 144.98°
Index ranges	$-9 \le h \le 9$, $-12 \le k \le 13$, $-15 \le l \le 14$
Reflections collected	9514
Independent reflections	3568 [R_{int} = 0.0297, R_{sigma} = 0.0249]
Data/restraints/parameters	3568/0/230
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0388, wR_2 = 0.1066
Final R indexes [all data]	R_1 = 0.0414, wR_2 = 0.1098
Largest diff. peak/hole / e Å^{-3}	0.69/ -0.49

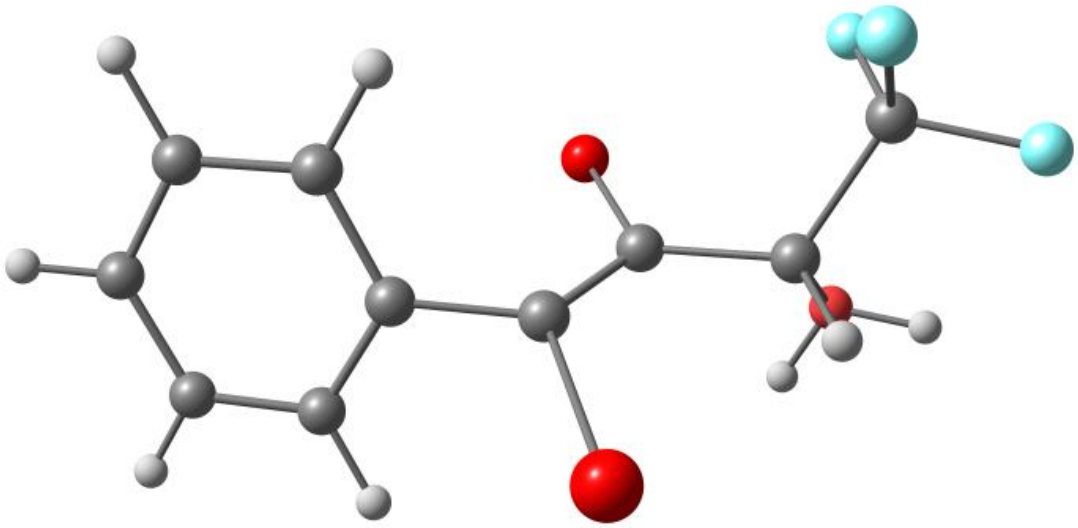
Optimized geometry, bond lengths, energy and Gibbs energy (T=298K), natural charges for structures **A1-A6**, **B1-B6**, **C1-C7**, **D1-D7**.

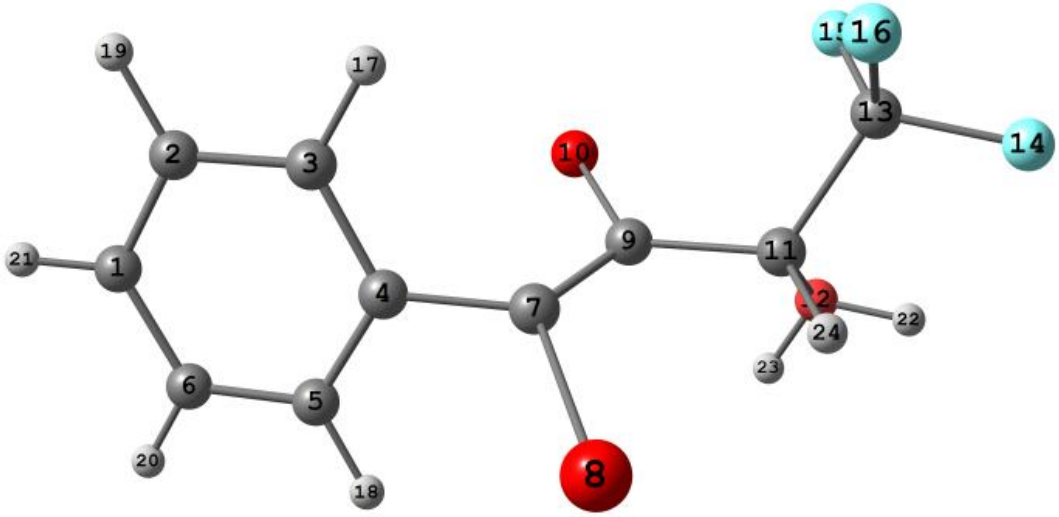
A1

E= -5908.91508704 h, G^{298}= -5908.799304 h μ= 9.96 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	4.571186	-0.913186	0.461078
2	C	3.588860	-1.165859	1.414106
3	C	2.295526	-0.694000	1.226772
4	C	1.983059	0.047724	0.083668
5	C	2.976253	0.317446	-0.863279
6	C	4.261534	-0.174185	-0.678095
7	C	0.615859	0.563141	-0.107135
8	Br	0.512515	2.488408	-0.063481
9	C	-0.494519	-0.172517	-0.278737
10	Br	-0.359082	-2.076328	-0.472199
11	C	-1.854194	0.402535	-0.384298
12	O	-2.468920	-0.015381	-1.720552
13	C	-2.910217	-0.007472	0.659255
14	F	-4.081697	0.575872	0.332488
15	F	-3.123081	-1.317484	0.748545
16	F	-2.519010	0.452250	1.847667
17	H	1.533790	-0.891688	1.967005
18	H	2.741165	0.900550	-1.742245
19	H	3.826939	-1.731165	2.303971
20	H	5.021402	0.024768	-1.420453
21	H	5.575105	-1.286424	0.606933
22	H	-3.323280	0.427029	-1.901291
23	H	-1.862172	0.152979	-2.468996
24	H	-1.817746	1.486700	-0.390018





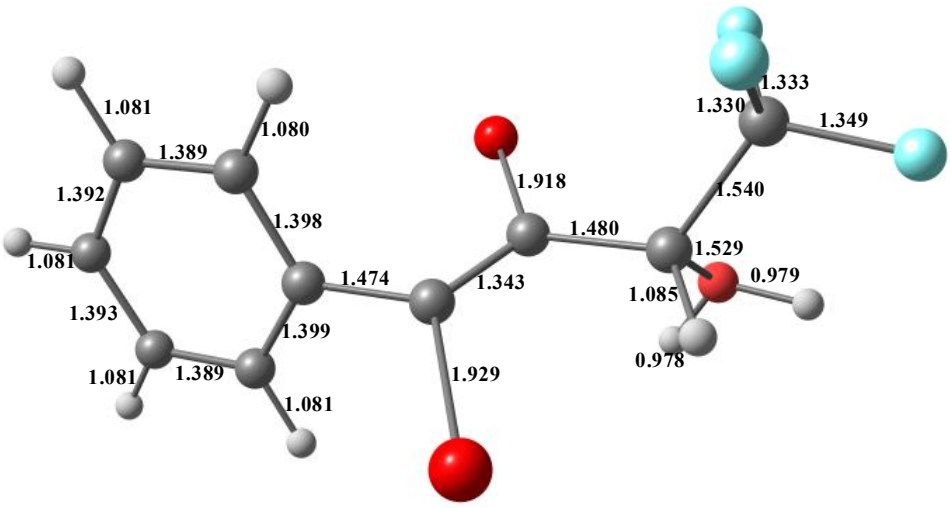
Natural charges, e

Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.18172	1.99915	4.16252	0.02004	6.18172
C	2	-0.19767	1.99915	4.17848	0.02005	6.19767
C	3	-0.16702	1.99903	4.14915	0.01883	6.16702
C	4	-0.12756	1.99885	4.10594	0.02277	6.12756
C	5	-0.16942	1.99903	4.15134	0.01904	6.16942
C	6	-0.19598	1.99915	4.17686	0.01996	6.19598
C	7	-0.01231	1.99831	3.97691	0.03710	6.01231

Br	8	0.13391	27.99906	6.85350	0.01353	34.86609
C	9	-0.23895	1.99823	4.20503	0.03569	6.23895
Br	10	0.14571	27.99906	6.84001	0.01522	34.85429
C	11	0.02933	1.99871	3.94354	0.02842	5.97067
O	12	-0.63346	1.99972	6.61576	0.01798	8.63346
C	13	1.07307	1.99928	2.87145	0.05620	4.92693
F	14	-0.35216	1.99992	7.34362	0.00863	9.35216
F	15	-0.33179	1.99991	7.32310	0.00878	9.33179
F	16	-0.32996	1.99991	7.32119	0.00886	9.32996
H	17	0.22583	0.00000	0.77236	0.00181	0.77417
H	18	0.22554	0.00000	0.77267	0.00179	0.77446
H	19	0.22170	0.00000	0.77661	0.00169	0.77830
H	20	0.22142	0.00000	0.77687	0.00170	0.77858
H	21	0.21938	0.00000	0.77907	0.00155	0.78062
H	22	0.58033	0.00000	0.41708	0.00260	0.41967
H	23	0.58253	0.00000	0.41520	0.00227	0.41747
H	24	0.27925	0.00000	0.71709	0.00366	0.72075
* Total *		1.00000	83.98649	87.64535	0.36816	172.00000

Bond lengths, Å

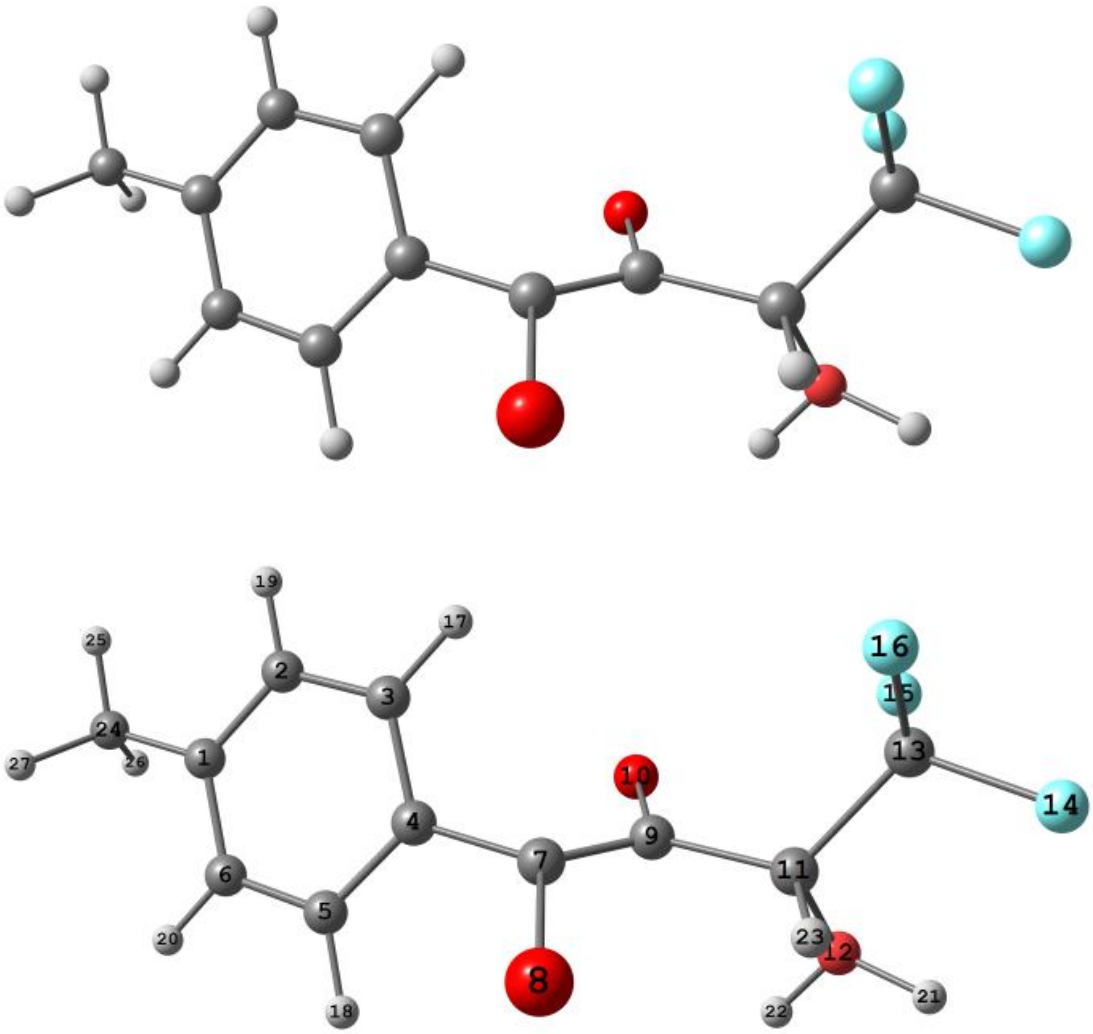


A2

E= -5948.24552031 h, G^{298}= -5948.106671 h μ= 10.14 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	4.391123	-0.487876	0.310966
2	C	3.420979	-0.920575	1.217033
3	C	2.087540	-0.560731	1.071715
4	C	1.694065	0.263174	0.014027
5	C	2.662979	0.725846	-0.884886
6	C	3.985718	0.340703	-0.742187
7	C	0.286563	0.657982	-0.133512
8	Br	0.011026	2.568940	-0.055323
9	C	-0.765233	-0.164549	-0.291801
10	Br	-0.486599	-2.044660	-0.560893
11	C	-2.171355	0.292618	-0.336641
12	O	-2.803603	-0.159490	-1.654705
13	C	-3.146060	-0.225487	0.737628
14	F	-4.367483	0.288935	0.490457
15	F	-3.266669	-1.550069	0.781577
16	F	-2.728882	0.213807	1.925443
17	H	1.356588	-0.908367	1.787161
18	H	2.377856	1.377221	-1.698678
19	H	3.709540	-1.548391	2.049262
20	H	4.718066	0.694680	-1.455580
21	H	-3.671337	0.258478	-1.826774
22	H	-2.215602	0.004828	-2.418503
23	H	-2.227872	1.375722	-0.325555
24	C	5.832031	-0.900545	0.451081
25	H	6.011800	-1.400044	1.400919
26	H	6.116027	-1.587225	-0.348959
27	H	6.496032	-0.038231	0.384062



Natural charges, e

Summary of Natural Population Analysis:

Natural Population

Natural ----------

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.00243	1.99905	3.98086	0.01766	5.99757
C	2	-0.20408	1.99904	4.18590	0.01915	6.20408
C	3	-0.15480	1.99904	4.13692	0.01884	6.15480
C	4	-0.14140	1.99884	4.12012	0.02244	6.14140
C	5	-0.15872	1.99904	4.14075	0.01893	6.15872
C	6	-0.19839	1.99904	4.18024	0.01911	6.19839
C	7	-0.00826	1.99832	3.97322	0.03672	6.00826
Br	8	0.12657	27.99908	6.86085	0.01350	34.87343
C	9	-0.24376	1.99824	4.20995	0.03557	6.24376

Br	10	0.14155	27.99906	6.84403	0.01535	34.85845
C	11	0.02902	1.99871	3.94377	0.02850	5.97098
O	12	-0.63485	1.99972	6.61713	0.01800	8.63485
C	13	1.07267	1.99928	2.87181	0.05624	4.92733
F	14	-0.35191	1.99992	7.34337	0.00862	9.35191
F	15	-0.33265	1.99991	7.32399	0.00876	9.33265
F	16	-0.33083	1.99991	7.32204	0.00888	9.33083
H	17	0.22489	0.00000	0.77321	0.00189	0.77511
H	18	0.22468	0.00000	0.77344	0.00187	0.77532
H	19	0.21885	0.00000	0.77915	0.00200	0.78115
H	20	0.21865	0.00000	0.77944	0.00190	0.78135
H	21	0.58044	0.00000	0.41700	0.00257	0.41956
H	22	0.58233	0.00000	0.41537	0.00229	0.41767
H	23	0.27912	0.00000	0.71719	0.00369	0.72088
C	24	-0.59575	1.99928	4.58441	0.01206	6.59575
H	25	0.21295	0.00000	0.78552	0.00153	0.78705
H	26	0.22204	0.00000	0.77639	0.00157	0.77796
H	27	0.21918	0.00000	0.77926	0.00156	0.78082

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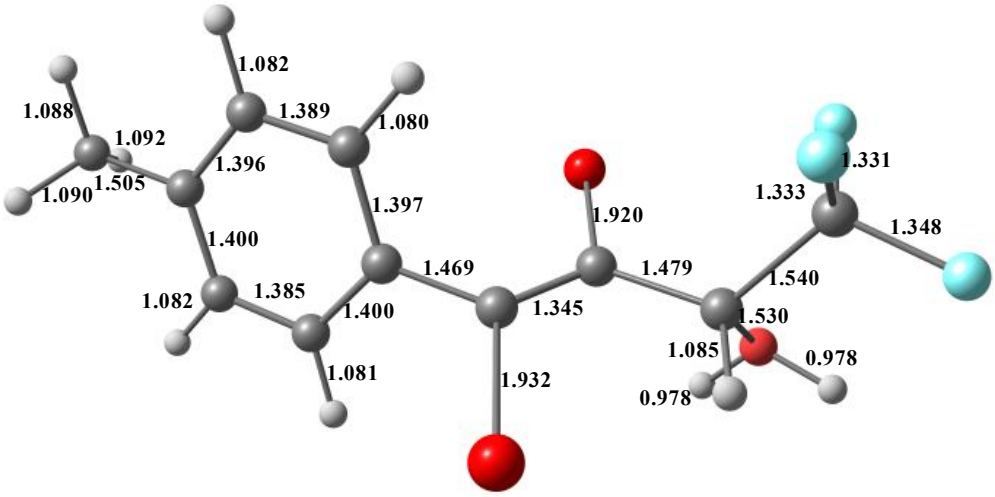
* Total *	1.00000	85.98547	93.63531	0.37922	180.00000

Bond lengths, Å

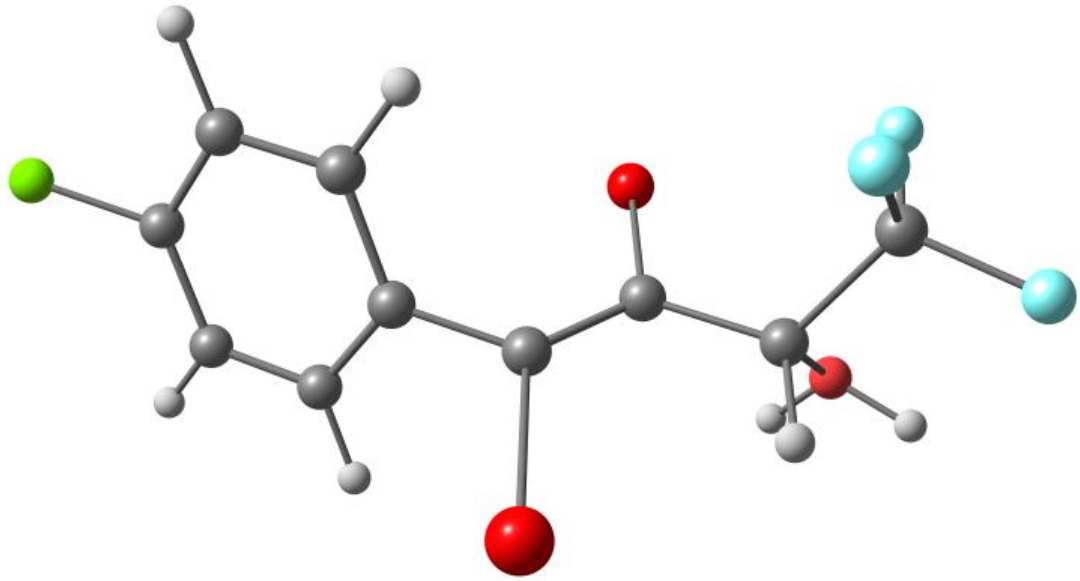


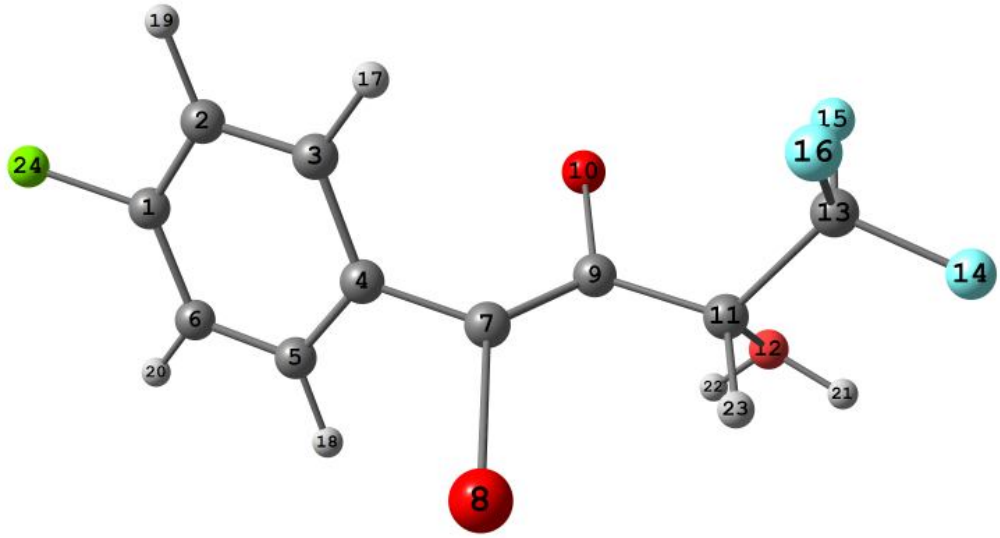
A3

E= -6368.53874127 h, G^{298}= -6368.434948 h μ= 13.88 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	4.105557	-0.257399	0.205176
2	C	3.220690	-0.680886	1.187493
3	C	1.873551	-0.370885	1.062658
4	C	1.417011	0.367753	-0.032093
5	C	2.328796	0.802548	-0.998326
6	C	3.673633	0.480853	-0.889525
7	C	-0.012312	0.704047	-0.154300
8	Br	-0.364830	2.596107	-0.053867
9	C	-1.021143	-0.168770	-0.303685
10	Br	-0.649346	-2.034438	-0.546820
11	C	-2.450469	0.219130	-0.345542
12	O	-3.073168	-0.297668	-1.639397
13	C	-3.383110	-0.320764	0.755882
14	F	-4.625980	0.148384	0.532032
15	F	-3.454275	-1.648735	0.809616
16	F	-2.955496	0.141567	1.930901
17	H	1.181835	-0.698440	1.824577
18	H	1.990171	1.385323	-1.842517
19	H	3.573859	-1.245243	2.036833
20	H	4.374807	0.804027	-1.643508
21	H	-3.941575	0.108375	-1.835191
22	H	-2.485069	-0.174285	-2.411104
23	H	-2.557923	1.298443	-0.360912
24	Cl	5.809055	-0.657647	0.352453





Natural charges, e

Summary of Natural Population Analysis:

Natural Population

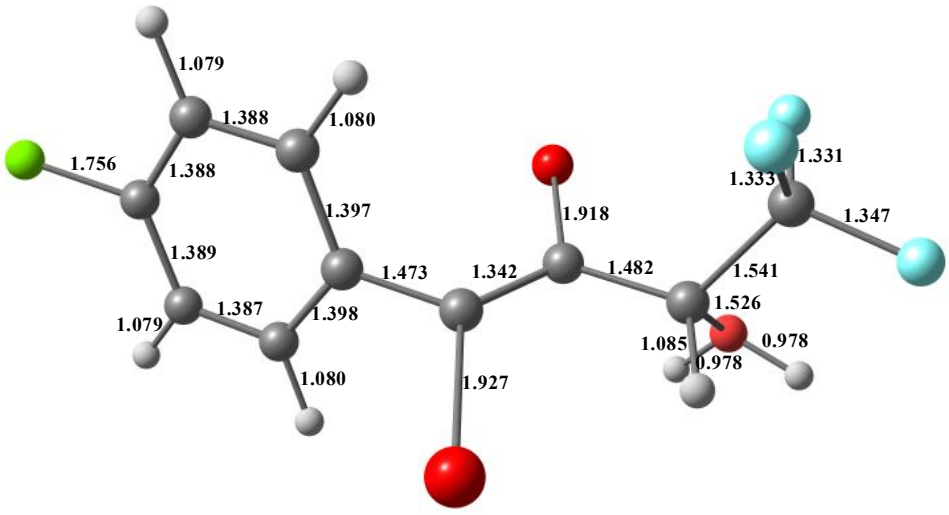
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.02432	1.99855	3.99824	0.02753	6.02432
C	2	-0.21964	1.99895	4.19871	0.02198	6.21964
C	3	-0.14736	1.99903	4.12976	0.01857	6.14736
C	4	-0.12508	1.99885	4.10385	0.02238	6.12508

C	5	-0.14903	1.99903	4.13125	0.01876	6.14903
C	6	-0.21775	1.99895	4.19688	0.02192	6.21775
C	7	-0.01927	1.99831	3.98395	0.03700	6.01927
Br	8	0.13866	27.99907	6.84871	0.01356	34.86134
C	9	-0.23657	1.99824	4.20246	0.03586	6.23657
Br	10	0.14837	27.99906	6.83732	0.01524	34.85163
C	11	0.03034	1.99872	3.94248	0.02846	5.96966
O	12	-0.63318	1.99972	6.61551	0.01794	8.63318
C	13	1.07306	1.99928	2.87136	0.05629	4.92694
F	14	-0.35045	1.99992	7.34191	0.00862	9.35045
F	15	-0.33270	1.99991	7.32405	0.00875	9.33270
F	16	-0.33053	1.99991	7.32172	0.00890	9.33053
H	17	0.23269	0.00000	0.76550	0.00181	0.76731
H	18	0.23239	0.00000	0.76582	0.00179	0.76761
H	19	0.23750	0.00000	0.76036	0.00214	0.76250
H	20	0.23724	0.00000	0.76060	0.00216	0.76276
H	21	0.58192	0.00000	0.41555	0.00253	0.41808
H	22	0.58344	0.00000	0.41427	0.00228	0.41656
H	23	0.27973	0.00000	0.71666	0.00361	0.72027
Cl	24	0.01053	9.99959	6.97177	0.01811	16.98947

==========

* Total *	1.00000	93.98508	93.61872	0.39621	188.00000

Bond lengths, Å

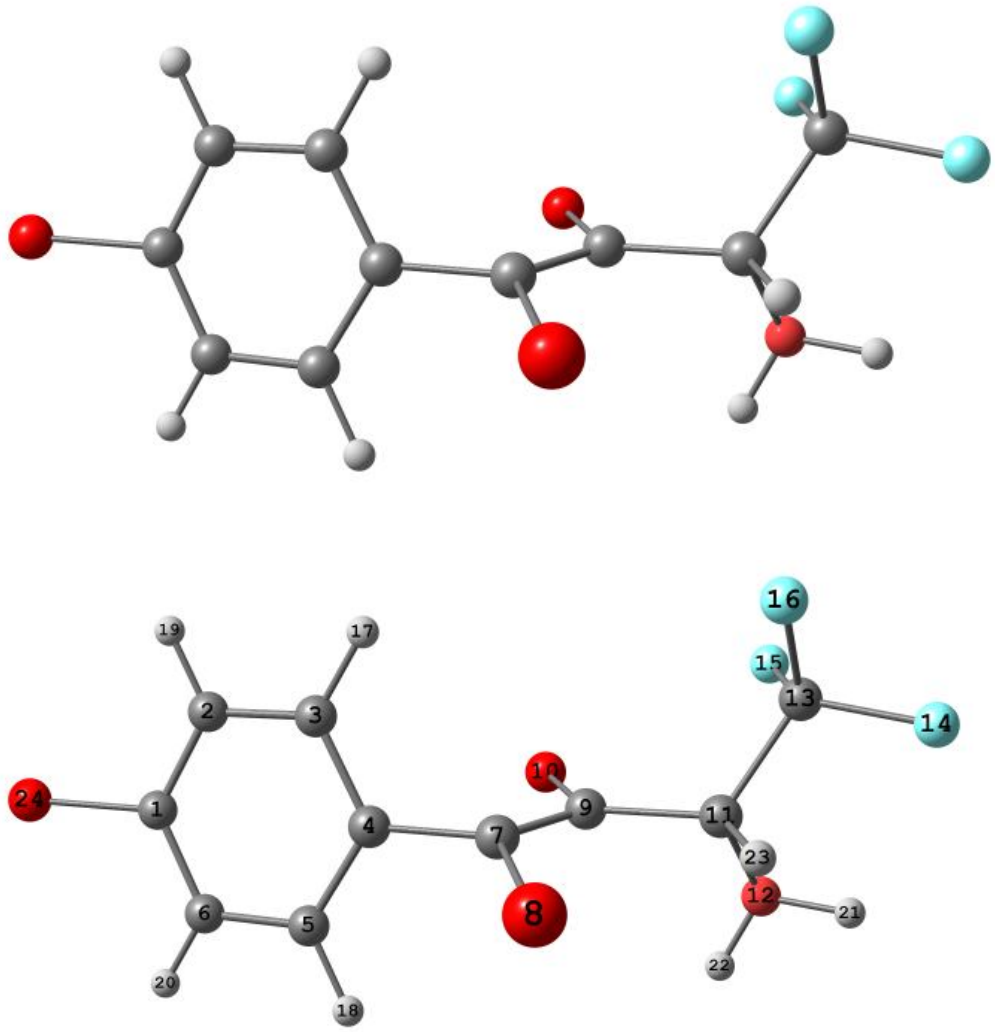


A4

E= -8482.45251182 h, G^{298}= -8482.352159 h μ= 16.41 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	3.581094	-0.038576	0.094250
2	C	2.773363	-0.302565	1.191454
3	C	1.409973	-0.051316	1.103803
4	C	0.864736	0.467338	-0.071976
5	C	1.696558	0.739757	-1.160303
6	C	3.057954	0.478299	-1.083528
7	C	-0.581546	0.746338	-0.158433
8	Br	-1.004047	2.622233	-0.051996
9	C	-1.550159	-0.172288	-0.285517
10	Br	-1.079381	-2.018505	-0.490083
11	C	-2.995027	0.153910	-0.330752
12	O	-3.580401	-0.356771	-1.644276
13	C	-3.919146	-0.442871	0.748101
14	F	-5.186653	-0.070479	0.472893
15	F	-3.896288	-1.770487	0.822562
16	F	-3.567258	0.066767	1.927659
17	H	0.775344	-0.256886	1.953540
18	H	1.284736	1.148018	-2.072007
19	H	3.192394	-0.699595	2.103058
20	H	3.695697	0.678108	-1.930768
21	H	-4.515869	-0.094853	-1.766851
22	H	-3.064564	-0.060628	-2.421270
23	H	-3.149173	1.227918	-0.322817
24	Br	5.461989	-0.391965	0.208384



Natural charges, e

Summary of Natural Population Analysis:

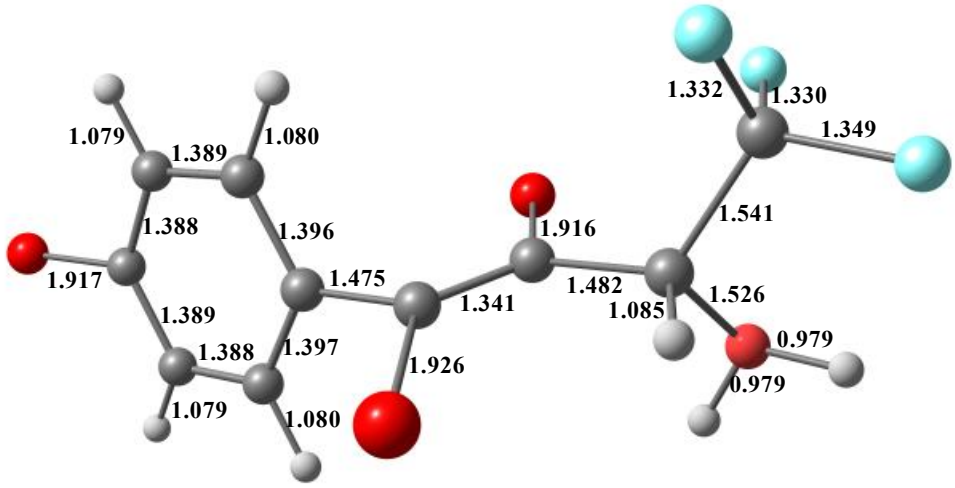
			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.09035	1.99858	4.06445	0.02733	6.09035
C	2	-0.22024	1.99894	4.19897	0.02234	6.22024
C	3	-0.15130	1.99902	4.13353	0.01874	6.15130
C	4	-0.12127	1.99885	4.09974	0.02269	6.12127
C	5	-0.15263	1.99902	4.13474	0.01887	6.15263
C	6	-0.21889	1.99894	4.19765	0.02230	6.21889
C	7	-0.01821	1.99830	3.98267	0.03724	6.01821
Br	8	0.14050	27.99906	6.84687	0.01357	34.85950
C	9	-0.23239	1.99822	4.19820	0.03597	6.23239

Br	10	0.15072	27.99905	6.83506	0.01518	34.84928
C	11	0.03040	1.99872	3.94255	0.02833	5.96960
O	12	-0.63229	1.99972	6.61470	0.01787	8.63229
C	13	1.07336	1.99929	2.87112	0.05623	4.92664
F	14	-0.35222	1.99992	7.34368	0.00863	9.35222
F	15	-0.33124	1.99991	7.32253	0.00880	9.33124
F	16	-0.32885	1.99991	7.32009	0.00886	9.32885
H	17	0.23280	0.00000	0.76542	0.00178	0.76720
H	18	0.23229	0.00000	0.76594	0.00177	0.76771
H	19	0.23692	0.00000	0.76095	0.00213	0.76308
H	20	0.23684	0.00000	0.76102	0.00214	0.76316
H	21	0.58072	0.00000	0.41668	0.00261	0.41928
H	22	0.58354	0.00000	0.41421	0.00225	0.41646
H	23	0.27940	0.00000	0.71702	0.00358	0.72060
Br	24	0.07242	27.99908	6.91321	0.01529	34.92758

==========

* Total *	1.00000	111.98451	93.62101	0.39448	206.00000

Bond lengths, Å

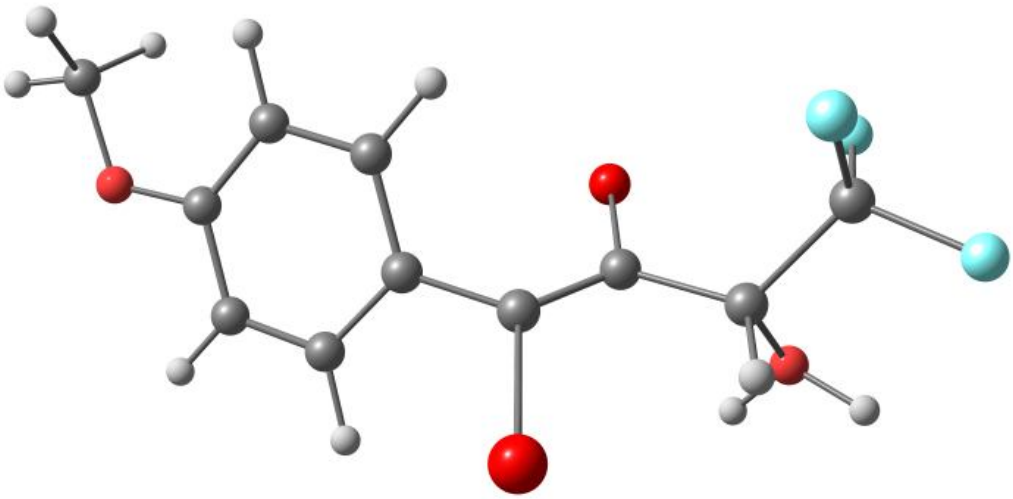


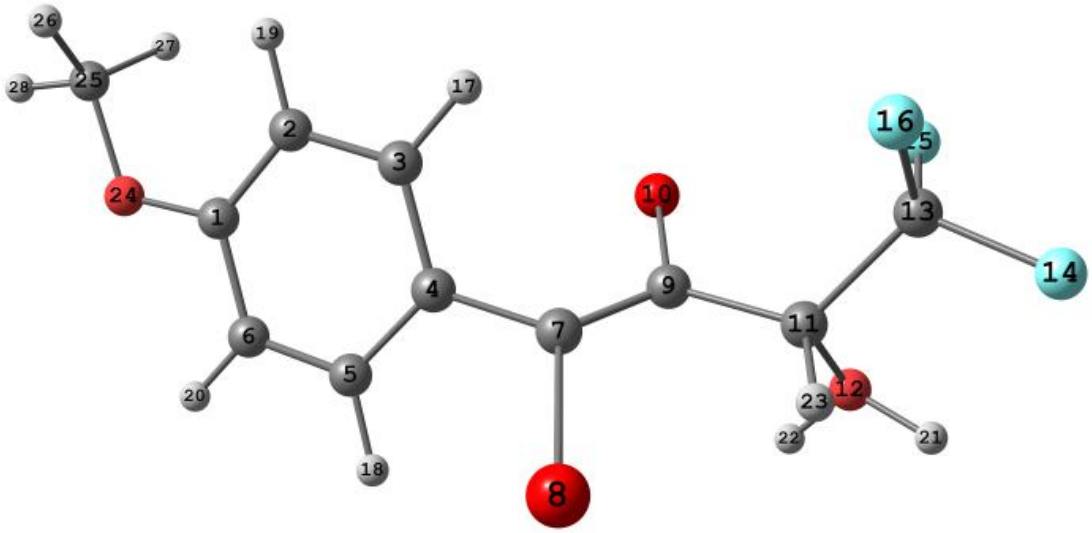
A5

E= -6023.47962671 h, G^{298}= -6023.33393 h μ= 9.15 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	4.164833	-0.127016	0.030116
2	C	3.276402	-0.786919	0.884363
3	C	1.919289	-0.507970	0.812721
4	C	1.422106	0.440448	-0.086669
5	C	2.329975	1.117751	-0.918681
6	C	3.676380	0.826457	-0.875074
7	C	-0.007442	0.741621	-0.129114
8	Br	-0.404186	2.627150	0.075753
9	C	-1.023536	-0.134543	-0.277306
10	Br	-0.661046	-1.962789	-0.742895
11	C	-2.444561	0.241376	-0.175718
12	O	-3.133433	0.021203	-1.540275
13	C	-3.358573	-0.510604	0.809115
14	F	-4.596104	0.021218	0.732648
15	F	-3.469359	-1.816725	0.580347
16	F	-2.888229	-0.321627	2.043194
17	H	1.245970	-1.020691	1.483340
18	H	1.972668	1.864375	-1.612707
19	H	3.626570	-1.510262	1.602837
20	H	4.372390	1.332202	-1.528467
21	H	-4.000443	0.470022	-1.605563
22	H	-2.568802	0.319134	-2.280585
23	H	-2.546374	1.298837	0.039870
24	O	5.500492	-0.331109	0.007696
25	C	6.068297	-1.286240	0.912503
26	H	5.890115	-0.995369	1.947642
27	H	5.664731	-2.282095	0.730505
28	H	7.134007	-1.281468	0.710484





Natural charges, e

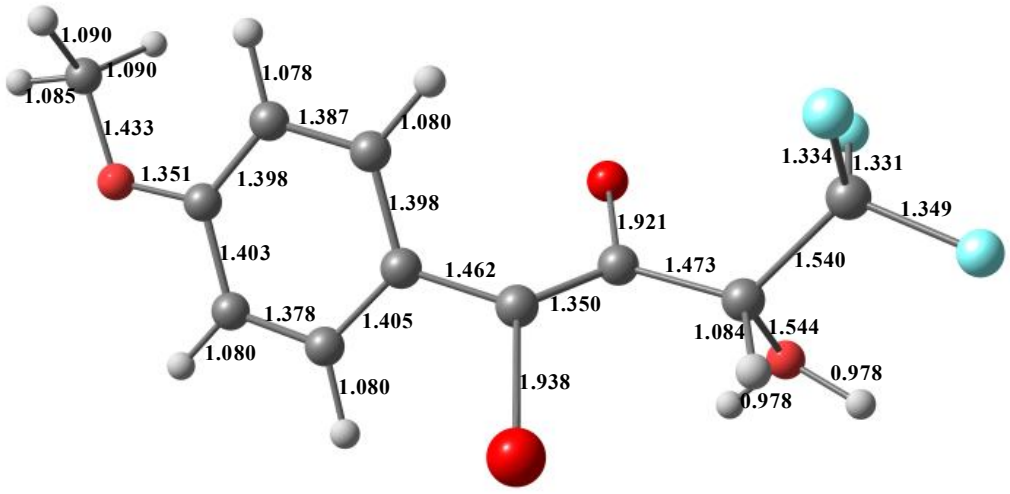
Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.35983	1.99881	3.61941	0.02194	5.64017
C	2	-0.28450	1.99904	4.26742	0.01804	6.28450
C	3	-0.13213	1.99906	4.11432	0.01875	6.13213
C	4	-0.16876	1.99884	4.14754	0.02239	6.16876
C	5	-0.14544	1.99906	4.12799	0.01839	6.14544
C	6	-0.24004	1.99905	4.22062	0.02036	6.24004
C	7	0.00139	1.99834	3.96378	0.03648	5.99861

Br	8	0.11890	27.99909	6.86859	0.01341	34.88110
C	9	-0.25348	1.99825	4.21992	0.03532	6.25348
Br	10	0.13588	27.99907	6.84954	0.01550	34.86412
C	11	0.02591	1.99870	3.94624	0.02915	5.97409
O	12	-0.63665	1.99973	6.62525	0.01167	8.63665
C	13	1.07303	1.99927	2.87143	0.05627	4.92697
F	14	-0.35298	1.99992	7.34443	0.00863	9.35298
F	15	-0.33287	1.99991	7.32417	0.00879	9.33287
F	16	-0.33169	1.99991	7.32292	0.00887	9.33169
H	17	0.22687	0.00000	0.77125	0.00189	0.77313
H	18	0.22743	0.00000	0.77075	0.00182	0.77257
H	19	0.23189	0.00000	0.76597	0.00214	0.76811
H	20	0.23022	0.00000	0.76761	0.00217	0.76978
H	21	0.57651	0.00000	0.42003	0.00346	0.42349
H	22	0.57859	0.00000	0.41823	0.00318	0.42141
H	23	0.27787	0.00000	0.71820	0.00392	0.72213
O	24	-0.54060	1.99970	6.51571	0.02519	8.54060
C	25	-0.20974	1.99923	4.19705	0.01346	6.20974
H	26	0.18249	0.00000	0.81532	0.00219	0.81751
H	27	0.18259	0.00000	0.81521	0.00220	0.81741
H	28	0.19948	0.00000	0.79928	0.00124	0.80052
==========						
* Total *		1.00000	87.98498	99.60820	0.40682	188.00000

Bond lengths, Å



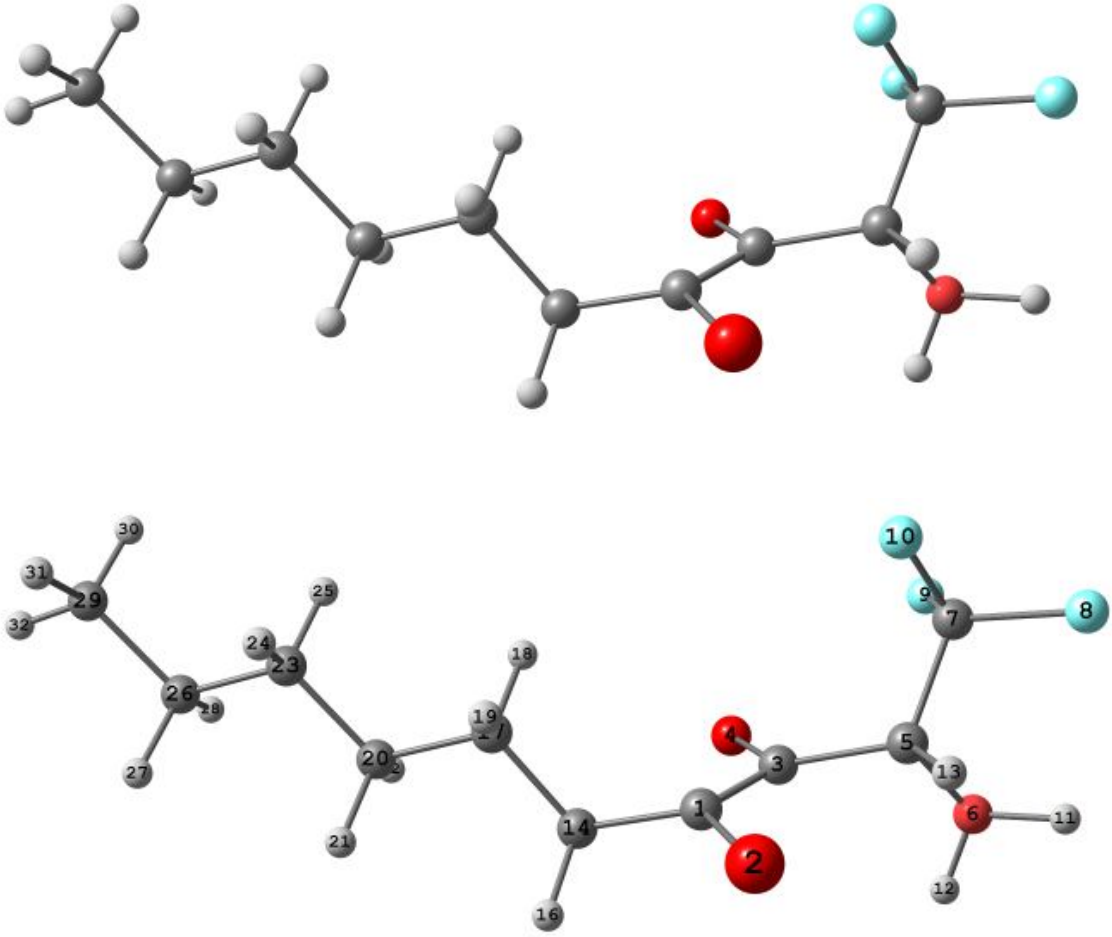
A6

E= -5913.7606632 h, G^{298}= -5913.562151 h μ= 13.33 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	0.109478	-0.669927	-0.681111
2	Br	0.286337	-2.551280	-0.324448
3	C	1.150659	0.154313	-0.476987
4	Br	0.968835	2.031693	-0.850264
5	C	2.474023	-0.290584	0.004462
6	O	3.533760	0.065229	-1.048871
7	C	3.032557	0.308614	1.308638
8	F	4.226234	-0.262339	1.565368
9	F	3.215268	1.626706	1.276813
10	F	2.193193	0.007907	2.300454
11	H	4.399201	-0.360783	-0.885739
12	H	3.235176	-0.166030	-1.950570
13	H	2.503380	-1.369844	0.110770
14	C	-1.260217	-0.290506	-1.137587
15	H	-1.208116	0.663013	-1.658851
16	H	-1.601569	-1.038638	-1.853045
17	C	-2.274411	-0.191932	0.021943
18	H	-1.936024	0.567906	0.729196
19	H	-2.299379	-1.139782	0.562070
20	C	-3.678815	0.150813	-0.479380
21	H	-3.999358	-0.608932	-1.198164
22	H	-3.648548	1.098556	-1.024657
23	C	-4.706855	0.246131	0.650384
24	H	-4.729552	-0.701122	1.198340
25	H	-4.386170	1.007167	1.368543
26	C	-6.119027	0.577772	0.161601
27	H	-6.436981	-0.180908	-0.559058
28	H	-6.097429	1.525818	-0.383184
29	C	-7.142688	0.664762	1.294789
30	H	-6.867234	1.437676	2.014956
31	H	-7.212011	-0.281118	1.835793

32	H	-8.136989	0.903527	0.915270



Natural charges, e

Summary of Natural Population Analysis:

Natural Population

Natural ----------

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.00961	1.99842	3.95622	0.03576	5.99039
Br	2	0.12801	27.99903	6.85875	0.01422	34.87199
C	3	-0.25956	1.99819	4.22551	0.03586	6.25956
Br	4	0.13173	27.99908	6.85381	0.01538	34.86827
C	5	0.02968	1.99871	3.94273	0.02888	5.97032
O	6	-0.63315	1.99973	6.62195	0.01147	8.63315
C	7	1.07224	1.99928	2.87217	0.05631	4.92776
F	8	-0.35173	1.99992	7.34314	0.00867	9.35173

F	9	-0.33313	1.99991	7.32443	0.00879	9.33313
F	10	-0.33106	1.99991	7.32219	0.00896	9.33106
H	11	0.57790	0.00000	0.41864	0.00346	0.42210
H	12	0.57952	0.00000	0.41732	0.00316	0.42048
H	13	0.27884	0.00000	0.71743	0.00373	0.72116
C	14	-0.44152	1.99909	4.41990	0.02253	6.44152
H	15	0.23835	0.00000	0.75894	0.00271	0.76165
H	16	0.23799	0.00000	0.75965	0.00235	0.76201
C	17	-0.36456	1.99925	4.34799	0.01731	6.36456
H	18	0.20222	0.00000	0.79548	0.00230	0.79778
H	19	0.20303	0.00000	0.79456	0.00242	0.79697
C	20	-0.37589	1.99927	4.35888	0.01774	6.37589
H	21	0.19346	0.00000	0.80397	0.00257	0.80654
H	22	0.19383	0.00000	0.80363	0.00254	0.80617
C	23	-0.37580	1.99927	4.35894	0.01759	6.37580
H	24	0.18963	0.00000	0.80789	0.00248	0.81037
H	25	0.18983	0.00000	0.80769	0.00248	0.81017
C	26	-0.37961	1.99931	4.36400	0.01630	6.37961
H	27	0.18777	0.00000	0.80972	0.00251	0.81223
H	28	0.18784	0.00000	0.80966	0.00250	0.81216
C	29	-0.57056	1.99936	4.56058	0.01063	6.57056
H	30	0.19286	0.00000	0.80518	0.00196	0.80714
H	31	0.19285	0.00000	0.80519	0.00196	0.80715
H	32	0.19939	0.00000	0.79914	0.00147	0.80061

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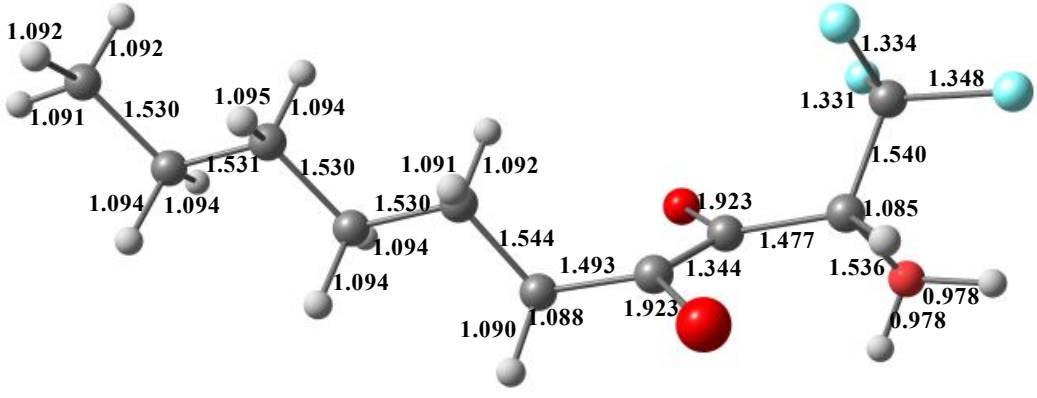
* Total *	1.00000	83.98770	95.64528	0.36701	180.00000

Bond lengths, Å

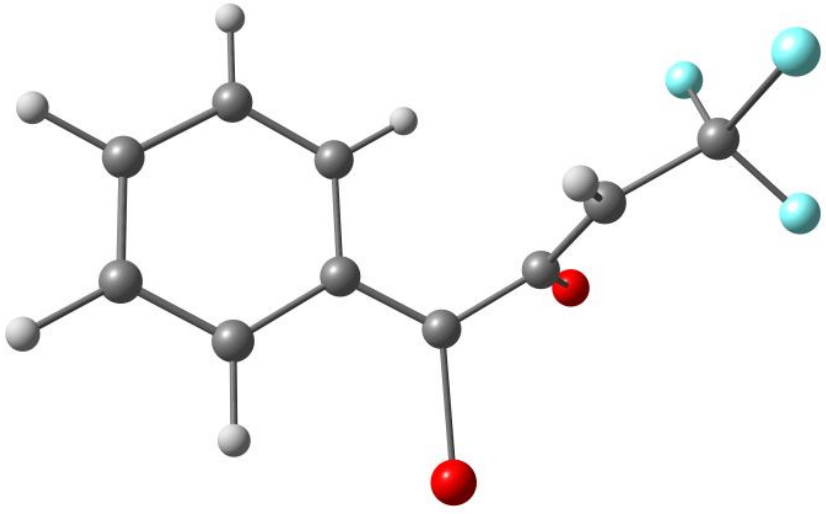


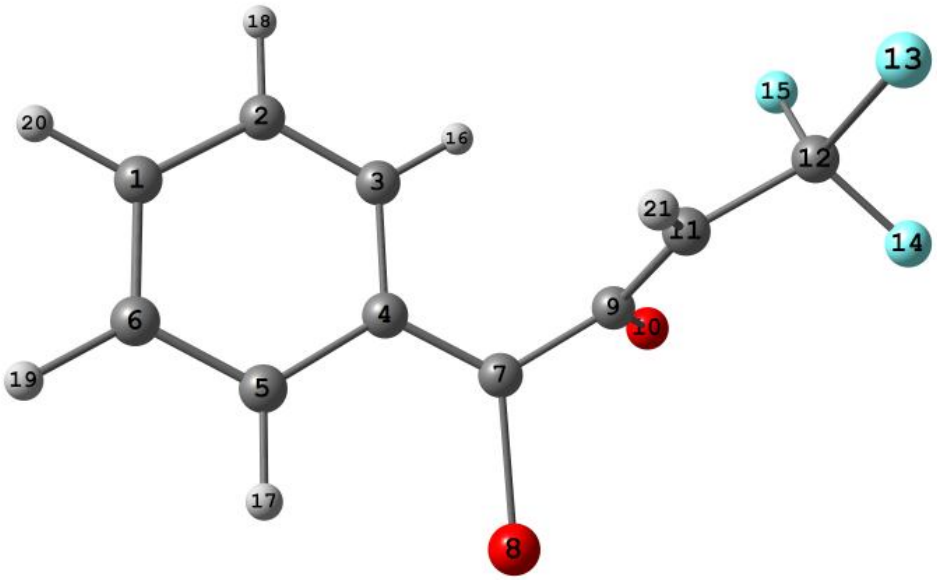
B1

E= -5832.4545732 h, G^{298}= -5832.365699 h μ= 12.12 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	3.931041	-2.299074	-0.443101
2	C	2.635087	-2.632965	-0.846524
3	C	1.605751	-1.746907	-0.638884
4	C	1.858544	-0.482420	-0.013769
5	C	3.197741	-0.163178	0.372190
6	C	4.207942	-1.065598	0.165632
7	C	0.799886	0.407554	0.180662
8	Br	1.076638	2.166604	0.727211
9	C	-0.608622	0.033325	0.001755
10	Br	-1.526772	0.990843	-1.360358
11	C	-1.166251	-0.892196	0.779317
12	C	-2.610466	-1.315760	0.752297
13	F	-2.826790	-2.245838	1.699119
14	F	-3.452908	-0.293377	0.993816
15	F	-2.963990	-1.856684	-0.429916
16	H	0.613198	-1.989765	-0.980389
17	H	3.404282	0.780999	0.849681
18	H	2.444526	-3.578652	-1.330337
19	H	5.215746	-0.830546	0.472120
20	H	4.736534	-3.000555	-0.608867
21	H	-0.570300	-1.385705	1.533328





Natural charges, e

Summary of Natural Population Analysis:

Natural Population

Natural ----------

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.02119	1.99918	4.00338	0.01862	6.02119
C	2	-0.20759	1.99914	4.18860	0.01985	6.20759
C	3	-0.05193	1.99908	4.03551	0.01734	6.05193
C	4	-0.16575	1.99877	4.14268	0.02430	6.16575
C	5	-0.06054	1.99907	4.04325	0.01822	6.06054
C	6	-0.19867	1.99915	4.18004	0.01948	6.19867
C	7	0.08876	1.99855	3.87512	0.03757	5.91124
Br	8	0.32732	27.99883	6.65953	0.01432	34.67268
C	9	-0.16001	1.99837	4.12573	0.03591	6.16001
Br	10	0.19426	27.99900	6.79149	0.01525	34.80574
C	11	-0.23438	1.99865	4.21066	0.02506	6.23438
C	12	1.06494	1.99928	2.88192	0.05387	4.93506
F	13	-0.34994	1.99992	7.34033	0.00970	9.34994
F	14	-0.34911	1.99991	7.33951	0.00969	9.34911
F	15	-0.34864	1.99991	7.33907	0.00965	9.34864
H	16	0.24116	0.00000	0.75685	0.00198	0.75884
H	17	0.24231	0.00000	0.75558	0.00211	0.75769

H	18	0.24351	0.00000	0.75491	0.00157	0.75649
H	19	0.24244	0.00000	0.75597	0.00158	0.75756
H	20	0.23553	0.00000	0.76312	0.00135	0.76447
H	21	0.26750	0.00000	0.73034	0.00216	0.73250

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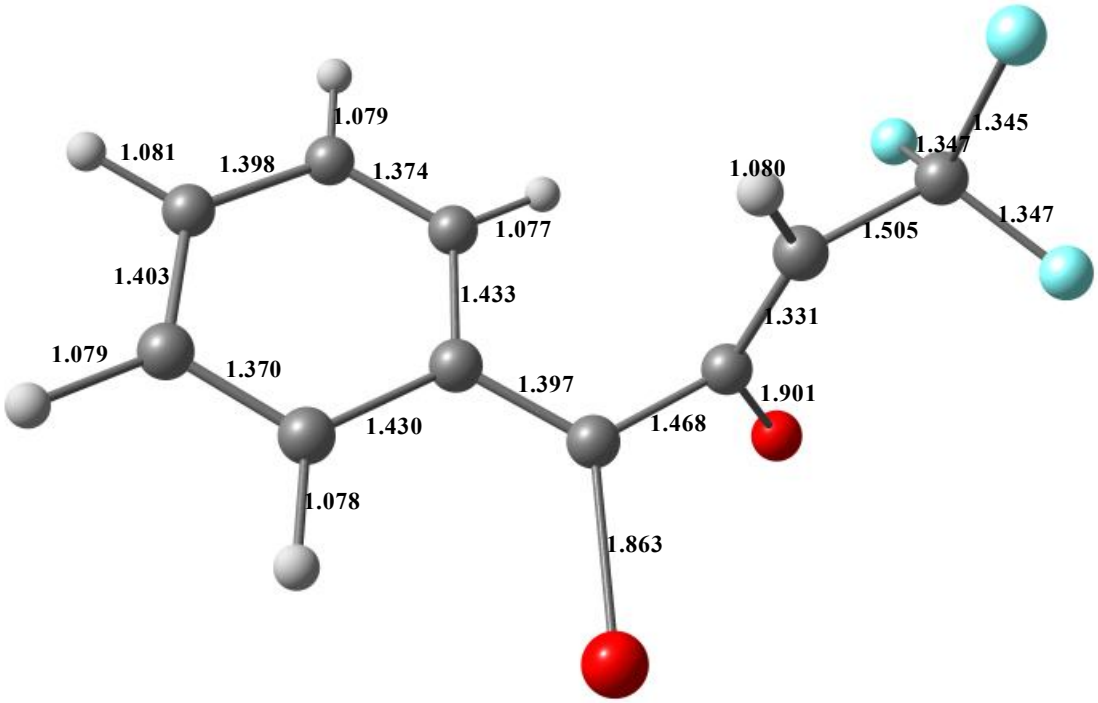
* Total *	1.00000	81.98681	79.67359	0.33959	162.00000

Bond lengths, Å

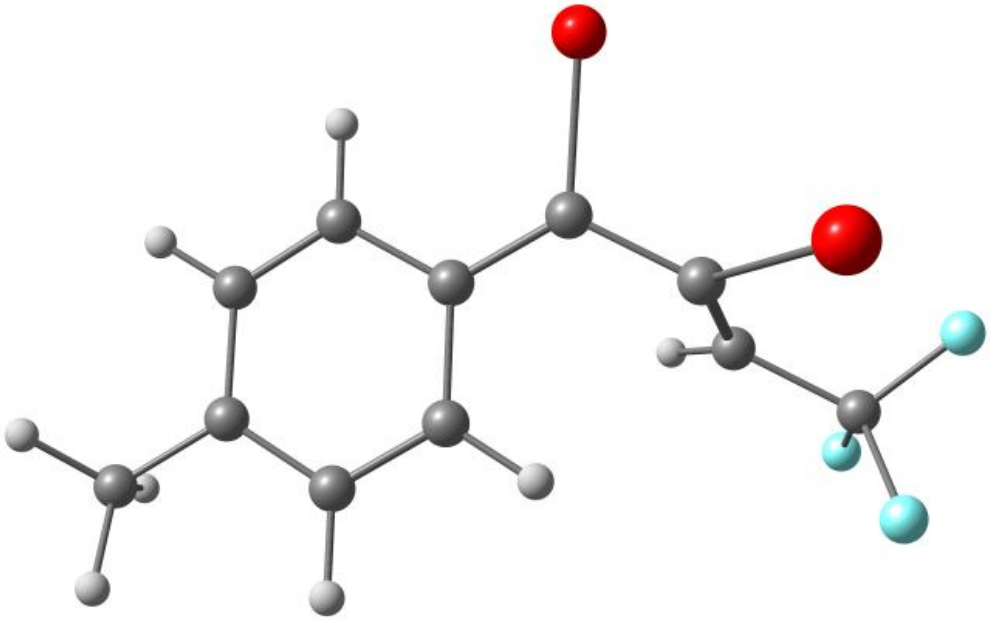


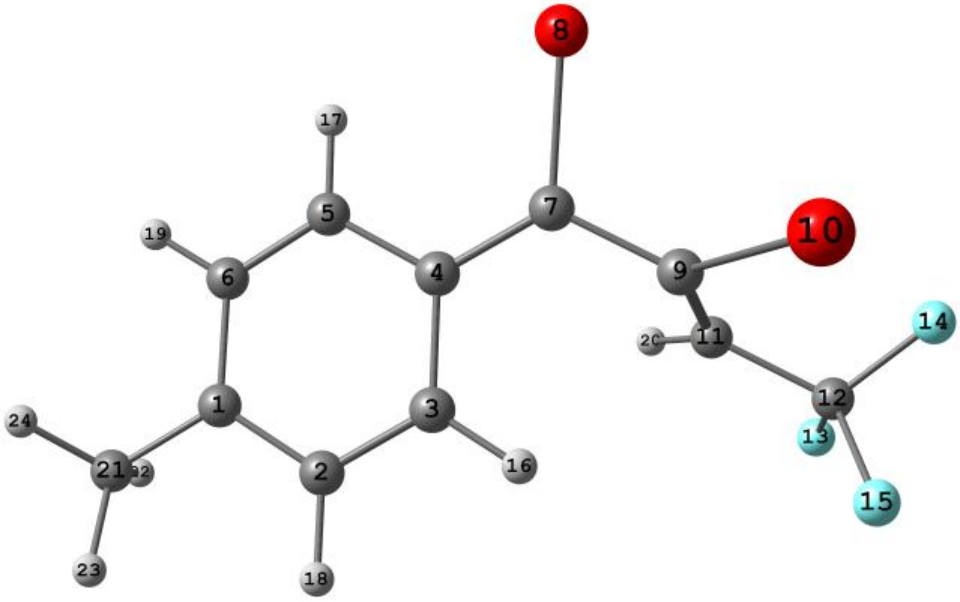
B2

E= -5871.79167332 h, G^{298}= -5871.677742 h μ= 13.12 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	4.107814	-1.278842	-0.208345
2	C	2.904294	-1.922219	-0.560788
3	C	1.700924	-1.288397	-0.417737
4	C	1.639425	0.052158	0.092307
5	C	2.871452	0.699840	0.432217
6	C	4.059448	0.044660	0.290096
7	C	0.408767	0.680093	0.220777
8	Br	0.251297	2.482807	0.692816
9	C	-0.876597	-0.005412	0.020324
10	Br	-1.843568	0.585985	-1.510024
11	C	-1.302195	-0.936725	0.867700
12	C	-2.616412	-1.663990	0.792976
13	F	-2.712383	-2.534880	1.814253
14	F	-3.673318	-0.831829	0.876010
15	F	-2.752805	-2.368937	-0.347521
16	H	0.795645	-1.789840	-0.718389
17	H	2.853814	1.707106	0.816407
18	H	2.936358	-2.924808	-0.961075
19	H	4.981016	0.540478	0.557834
20	H	-0.688431	-1.205399	1.715694
21	C	5.411535	-1.982302	-0.339394
22	H	5.663070	-2.436979	0.625313
23	H	5.368468	-2.780617	-1.076101
24	H	6.215375	-1.290043	-0.582879





Natural charges, e

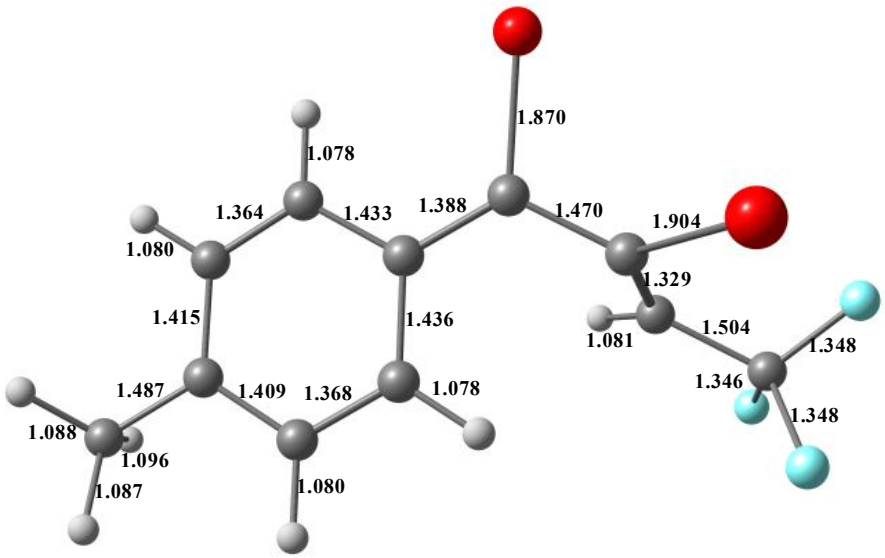
Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.16990	1.99909	3.81416	0.01685	5.83010
C	2	-0.21156	1.99902	4.19280	0.01974	6.21156
C	3	-0.04704	1.99908	4.03080	0.01716	6.04704

C	4	-0.16255	1.99876	4.13992	0.02386	6.16255
C	5	-0.05719	1.99907	4.04010	0.01803	6.05719
C	6	-0.20092	1.99903	4.18244	0.01946	6.20092
C	7	0.07163	1.99852	3.89308	0.03676	5.92837
Br	8	0.29840	27.99886	6.68852	0.01422	34.70160
C	9	-0.15117	1.99837	4.11728	0.03551	6.15117
Br	10	0.18627	27.99900	6.79952	0.01521	34.81373
C	11	-0.25089	1.99863	4.22712	0.02514	6.25089
C	12	1.06575	1.99927	2.88112	0.05386	4.93425
F	13	-0.35144	1.99992	7.34185	0.00968	9.35144
F	14	-0.35092	1.99991	7.34135	0.00966	9.35092
F	15	-0.35045	1.99991	7.34087	0.00967	9.35045
H	16	0.24092	0.00000	0.75706	0.00202	0.75908
H	17	0.24264	0.00000	0.75525	0.00211	0.75736
H	18	0.24121	0.00000	0.75692	0.00188	0.75879
H	19	0.24027	0.00000	0.75789	0.00184	0.75973
H	20	0.26693	0.00000	0.73092	0.00215	0.73307
C	21	-0.62009	1.99926	4.60651	0.01432	6.62009
H	22	0.25984	0.00000	0.73863	0.00152	0.74016
H	23	0.23336	0.00000	0.76505	0.00159	0.76664
H	24	0.23710	0.00000	0.76128	0.00162	0.76290

Bond lengths, Å

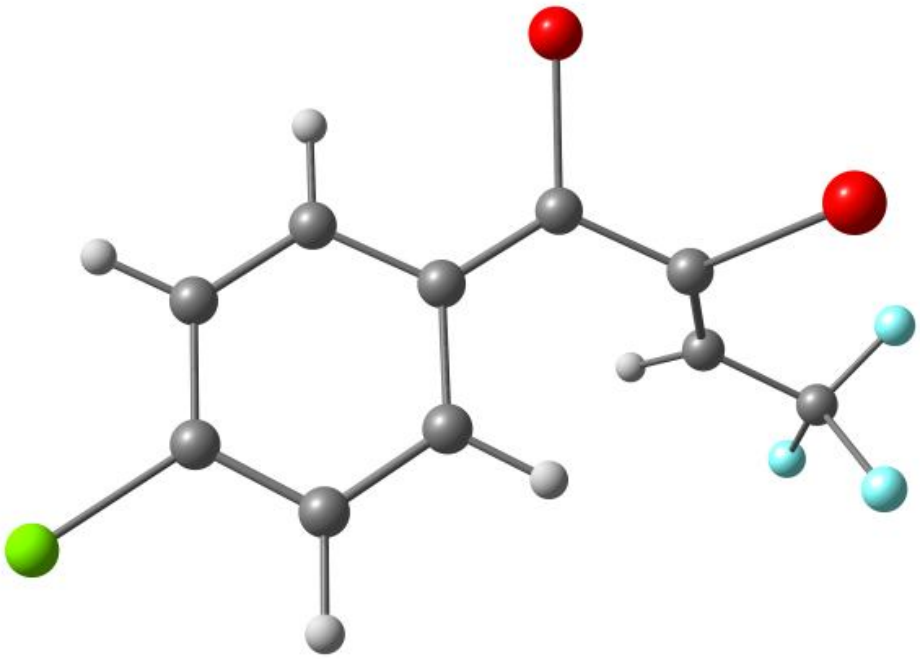


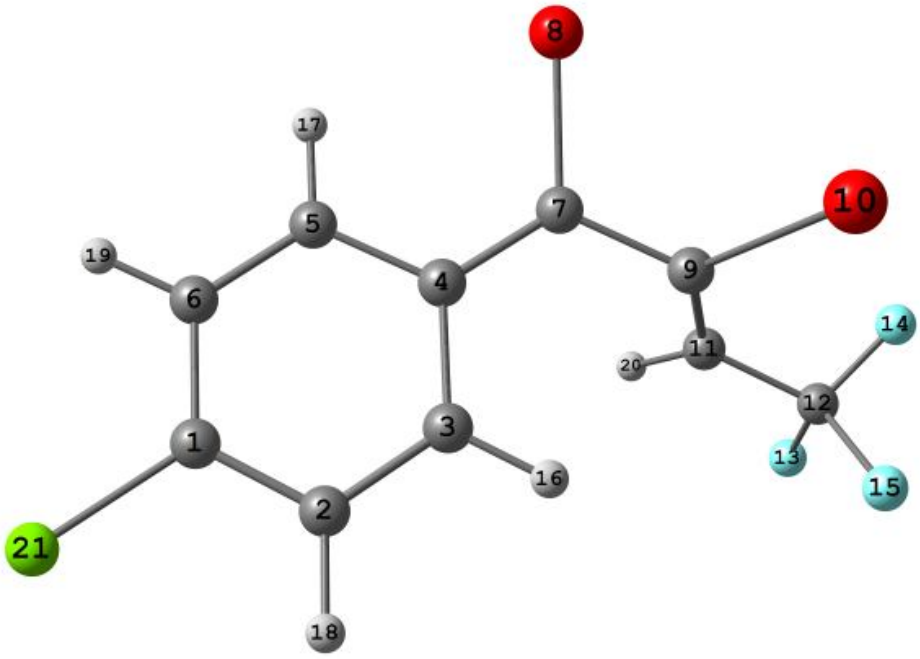
B3

E= -6292.07859384 h, G^{298}= -6292.001394 h μ= 9.49 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	3.934267	-0.731148	-0.138389
2	C	2.846117	-1.515555	-0.543232
3	C	1.579429	-1.009140	-0.426479
4	C	1.361829	0.305417	0.101783
5	C	2.502290	1.079372	0.484642
6	C	3.763555	0.566888	0.374494
7	C	0.062074	0.795532	0.214505
8	Br	-0.287899	2.569276	0.672718
9	C	-1.131428	-0.035891	0.012439
10	Br	-2.234456	0.494586	-1.444128
11	C	-1.396544	-1.055657	0.825279
12	C	-2.609845	-1.943971	0.761945
13	F	-2.540510	-2.875062	1.730085
14	F	-3.757555	-1.262308	0.941809
15	F	-2.710265	-2.594973	-0.413142
16	H	0.744928	-1.599762	-0.766483
17	H	2.364952	2.070627	0.885373
18	H	3.010816	-2.499664	-0.952074
19	H	4.623248	1.143470	0.676893
20	H	-0.719518	-1.280671	1.636682
21	Cl	5.521323	-1.365478	-0.283043





Natural charges, e

Summary of Natural Population Analysis:

Natural Population

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.07478	1.99868	3.89697	0.02957	5.92522
C	2	-0.22364	1.99895	4.20188	0.02281	6.22364

C	3	-0.04523	1.99908	4.02910	0.01705	6.04523
C	4	-0.16181	1.99877	4.13918	0.02385	6.16181
C	5	-0.05140	1.99907	4.03440	0.01793	6.05140
C	6	-0.21439	1.99896	4.19294	0.02248	6.21439
C	7	0.07637	1.99854	3.88787	0.03722	5.92363
Br	8	0.31777	27.99884	6.66905	0.01434	34.68223
C	9	-0.15675	1.99837	4.12263	0.03575	6.15675
Br	10	0.19147	27.99900	6.79429	0.01524	34.80853
C	11	-0.23918	1.99864	4.21543	0.02511	6.23918
C	12	1.06508	1.99928	2.88176	0.05388	4.93492
F	13	-0.35031	1.99992	7.34071	0.00969	9.35031
F	14	-0.34948	1.99991	7.33989	0.00968	9.34948
F	15	-0.34905	1.99991	7.33946	0.00968	9.34905
H	16	0.24713	0.00000	0.75087	0.00200	0.75287
H	17	0.24842	0.00000	0.74945	0.00213	0.75158
H	18	0.25661	0.00000	0.74135	0.00204	0.74339
H	19	0.25577	0.00000	0.74219	0.00204	0.74423
H	20	0.26732	0.00000	0.73053	0.00216	0.73268
Cl	21	0.14051	9.99951	6.84142	0.01857	16.85949

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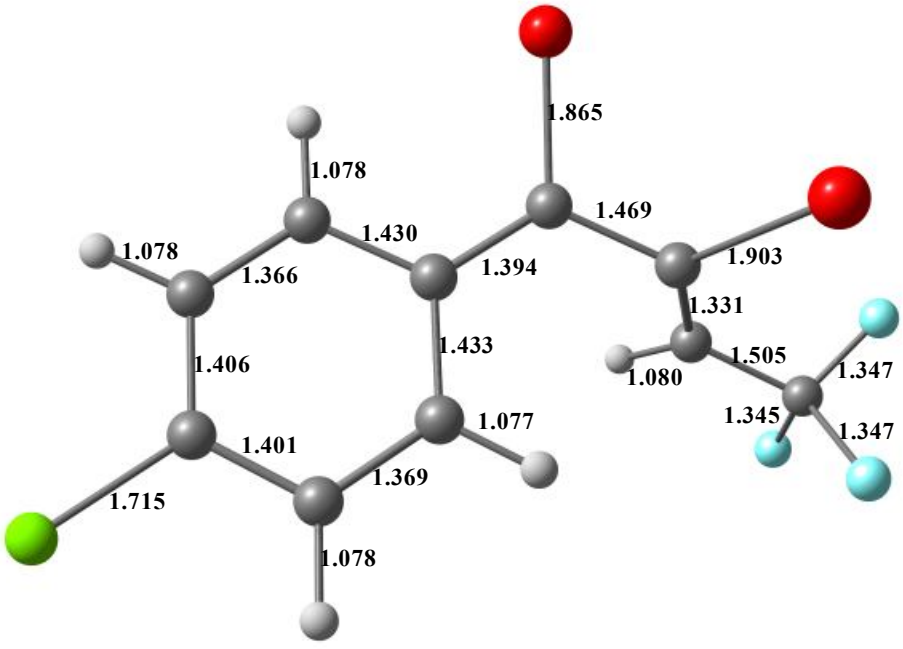
* Total *	1.00000	91.98543	85.64136	0.373211	78.00000

Bond lengths, Å

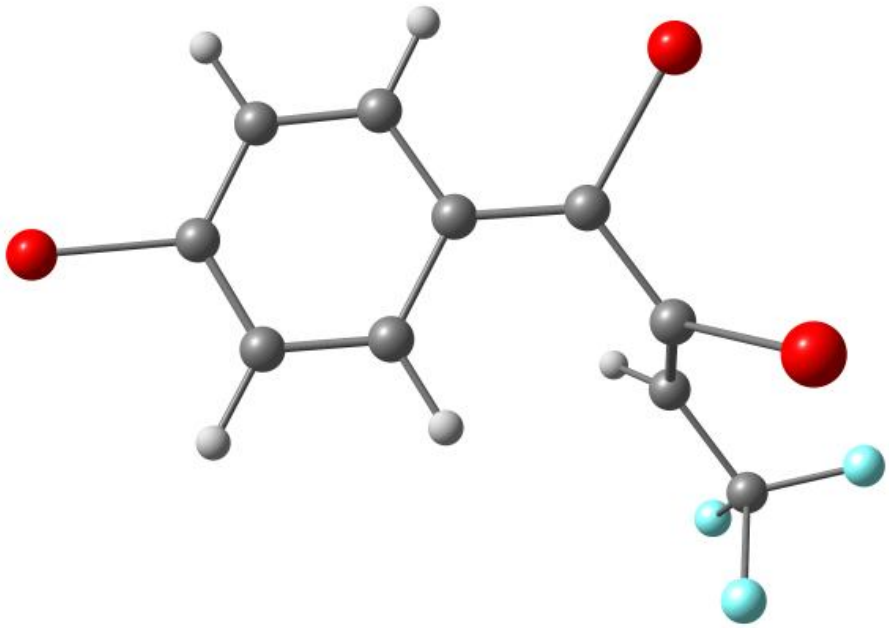


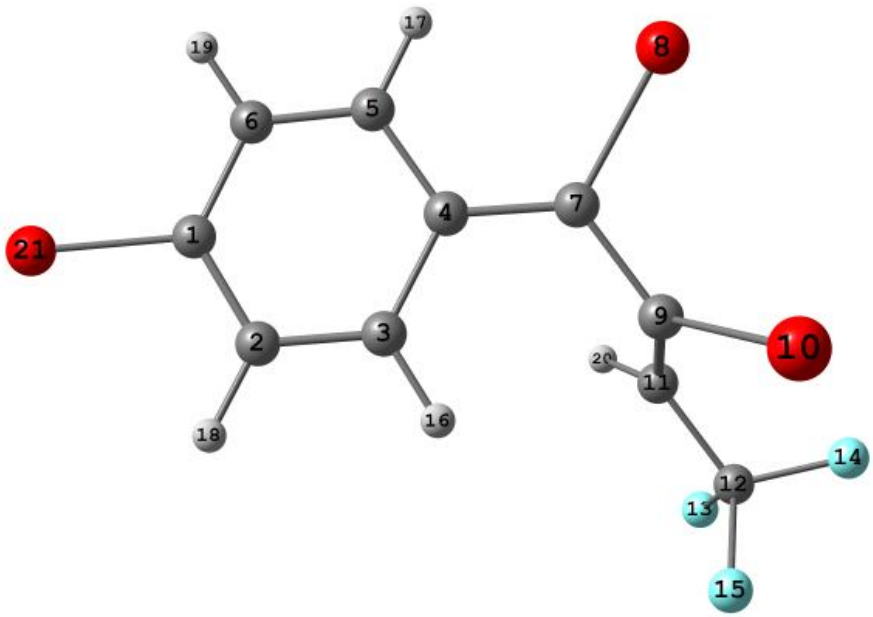
B4

E= -8405.99233387 h, G^{298}= -8405.916413 h μ= 7.68 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	3.450119	-0.253850	-0.038941
2	C	2.452208	-1.155648	-0.429842
3	C	1.138649	-0.778715	-0.337053
4	C	0.781459	0.521018	0.149352
5	C	1.832520	1.417145	0.520902
6	C	3.141017	1.032649	0.435359
7	C	-0.562728	0.877600	0.231666
8	Br	-1.103454	2.612281	0.653273
9	C	-1.664098	-0.071156	0.016908
10	Br	-2.732222	0.301434	-1.513639
11	C	-1.878501	-1.076495	0.860684
12	C	-3.003702	-2.072384	0.781006
13	F	-2.889065	-2.965999	1.779867
14	F	-4.213823	-1.491426	0.899173
15	F	-3.003030	-2.762432	-0.375756
16	H	0.372200	-1.463309	-0.660689
17	H	1.592158	2.401259	0.889860
18	H	2.715004	-2.131019	-0.806933
19	H	3.930022	1.706307	0.729070
20	H	-1.227545	-1.206020	1.713417
21	Br	5.248526	-0.769987	-0.160620





Natural charges, e

Summary of Natural Population Analysis:

Natural Population

Natural ----------

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.00182	1.99871	3.97026	0.02921	5.99818
C	2	-0.22712	1.99894	4.20484	0.02334	6.22712
C	3	-0.04441	1.99907	4.02819	0.01715	6.04441

C	4	-0.16178	1.99877	4.13899	0.02402	6.16178
C	5	-0.05145	1.99906	4.03435	0.01803	6.05145
C	6	-0.21791	1.99895	4.19594	0.02303	6.21791
C	7	0.07553	1.99854	3.88877	0.03716	5.92447
Br	8	0.31683	27.99884	6.66996	0.01437	34.68317
C	9	-0.15580	1.99837	4.12176	0.03567	6.15580
Br	10	0.19121	27.99900	6.79456	0.01523	34.80879
C	11	-0.24392	1.99864	4.22012	0.02516	6.24392
C	12	1.06543	1.99928	2.88141	0.05388	4.93457
F	13	-0.35063	1.99992	7.34103	0.00969	9.35063
F	14	-0.35014	1.99991	7.34056	0.00966	9.35014
F	15	-0.34934	1.99991	7.33974	0.00968	9.34934
H	16	0.24679	0.00000	0.75120	0.00201	0.75321
H	17	0.24828	0.00000	0.74959	0.00213	0.75172
H	18	0.25575	0.00000	0.74223	0.00203	0.74425
H	19	0.25478	0.00000	0.74318	0.00204	0.74522
H	20	0.26748	0.00000	0.73038	0.00214	0.73252
Br	21	0.22861	27.99892	6.75729	0.01518	34.77139

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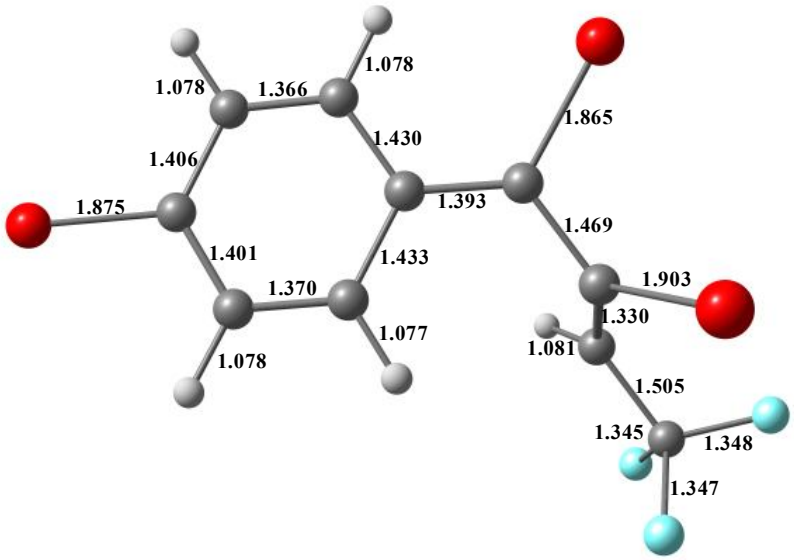
* Total *	1.00000	109.98483	85.64437	0.37080	196.00000

Bond lengths, Å

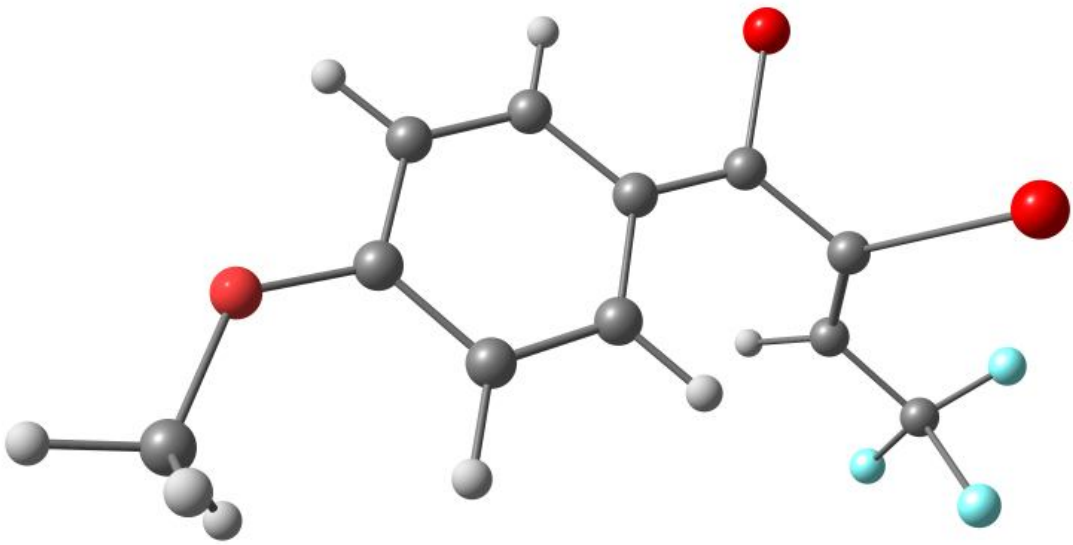


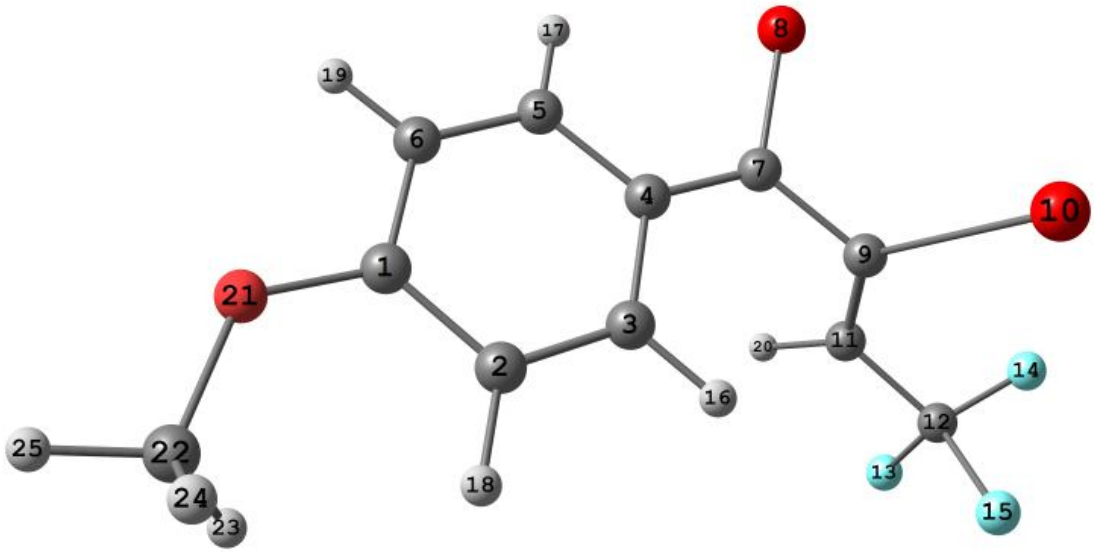
B5

E= -5947.0361756 h, G^{298}= -5946.917542 h μ= 14.04 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	3.996797	-0.495749	0.005408
2	C	2.929067	-1.376396	-0.308937
3	C	1.648074	-0.926697	-0.227273
4	C	1.347975	0.426869	0.166345
5	C	2.455821	1.297610	0.464682
6	C	3.731114	0.849902	0.393737
7	C	0.036906	0.843139	0.228271
8	Br	-0.435770	2.624853	0.603841
9	C	-1.119442	-0.044273	0.025559
10	Br	-2.032647	0.245714	-1.624070
11	C	-1.480706	-0.940442	0.936391
12	C	-2.661290	-1.866395	0.853715
13	F	-2.745194	-2.595566	1.982599
14	F	-3.831426	-1.211858	0.715411
15	F	-2.568590	-2.734482	-0.174787
16	H	0.842360	-1.596529	-0.480412
17	H	2.262261	2.316218	0.760083
18	H	3.124040	-2.390085	-0.617226
19	H	4.569223	1.489402	0.625054
20	H	-0.905948	-1.030375	1.847205
21	O	5.259874	-0.825646	-0.037909
22	C	5.674609	-2.162943	-0.422149
23	H	5.258071	-2.891555	0.267754
24	H	5.364258	-2.364410	-1.443838
25	H	6.754660	-2.147955	-0.350832





Natural charges, e

Summary of Natural Population Analysis:

Natural Population

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.49313	1.99896	3.48563	0.02229	5.50687
C	2	-0.27172	1.99904	4.25480	0.01789	6.27172
C	3	-0.04403	1.99909	4.02757	0.01737	6.04403
C	4	-0.15792	1.99874	4.13534	0.02384	6.15792
C	5	-0.07606	1.99907	4.05917	0.01782	6.07606
C	6	-0.22045	1.99904	4.20100	0.02041	6.22045

C	7	0.03885	1.99849	3.92691	0.03575	5.96115
Br	8	0.25607	27.99891	6.73092	0.01411	34.74393
C	9	-0.14007	1.99838	4.10671	0.03498	6.14007
Br	10	0.17280	27.99901	6.81300	0.01520	34.82720
C	11	-0.26372	1.99862	4.23996	0.02514	6.26372
C	12	1.06616	1.99927	2.88078	0.05380	4.93384
F	13	-0.35321	1.99992	7.34364	0.00966	9.35321
F	14	-0.35213	1.99991	7.34255	0.00967	9.35213
F	15	-0.35244	1.99991	7.34289	0.00963	9.35244
H	16	0.24286	0.00000	0.75512	0.00202	0.75714
H	17	0.24486	0.00000	0.75306	0.00208	0.75514
H	18	0.25149	0.00000	0.74653	0.00198	0.74851
H	19	0.25065	0.00000	0.74733	0.00201	0.74935
H	20	0.26559	0.00000	0.73228	0.00213	0.73441
O	21	-0.45548	1.99967	6.43082	0.02500	8.45548
C	22	-0.21503	1.99920	4.20368	0.01215	6.21503
H	23	0.20245	0.00000	0.79584	0.00171	0.79755
H	24	0.20300	0.00000	0.79530	0.00170	0.79700
H	25	0.21435	0.00000	0.78453	0.00111	0.78565

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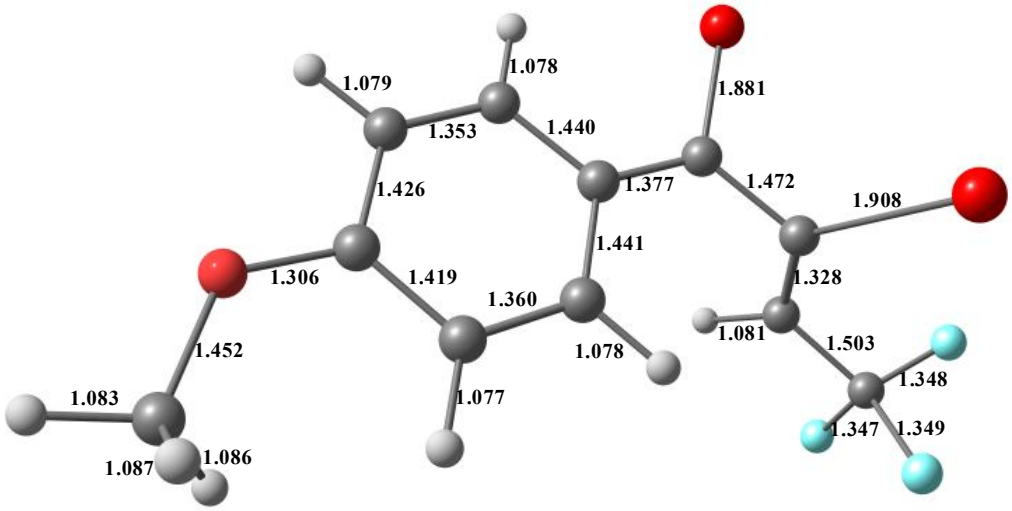
* Total *	1.00000	85.98522	91.63536	0.37942	178.00000

Bond lengths, Å

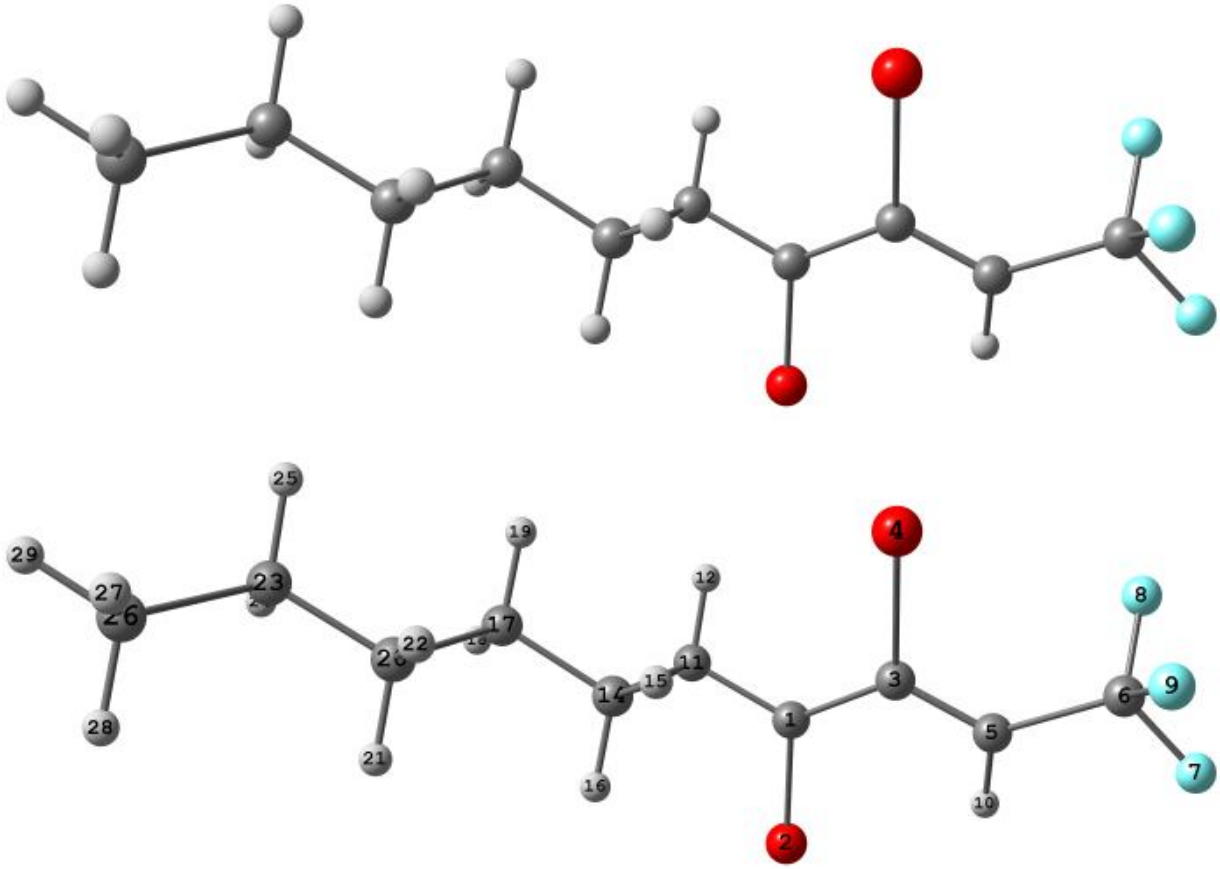


B6

E=-5837.28246106 h, G^{298}= -5837.109757 h μ= 5.77 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	-0.213676	0.940879	-0.486914
2	Br	-0.474190	2.703220	-0.005216
3	C	-1.236230	-0.040241	-0.197206
4	Br	-0.776790	-1.867840	-0.472779
5	C	-2.468435	0.318674	0.211150
6	C	-3.627774	-0.610449	0.491888
7	F	-4.682567	0.106741	0.904017
8	F	-3.995838	-1.287791	-0.606774
9	F	-3.334541	-1.497709	1.454646
10	H	-2.703950	1.362681	0.353721
11	C	1.070473	0.622074	-1.087650
12	H	0.993081	-0.269928	-1.704057
13	H	1.441356	1.461598	-1.668781
14	C	2.126557	0.337108	0.065921
15	H	1.744316	-0.439528	0.725509
16	H	2.237495	1.250626	0.647803
17	C	3.460144	-0.088478	-0.547407
18	H	3.801554	0.677010	-1.247534
19	H	3.323347	-1.007832	-1.120403
20	C	4.520706	-0.307395	0.537671
21	H	4.647763	0.615031	1.111009
22	H	4.168719	-1.065488	1.242893
23	C	5.875065	-0.738107	-0.035248
24	H	6.221003	0.016668	-0.746339
25	H	5.746959	-1.661982	-0.605346
26	C	6.935670	-0.945918	1.047058
27	H	6.629746	-1.718555	1.754779
28	H	7.106251	-0.027538	1.611738
29	H	7.888159	-1.251096	0.612225



Natural charges, e

Summary of Natural Population Analysis:

Natural Population

Natural ----------

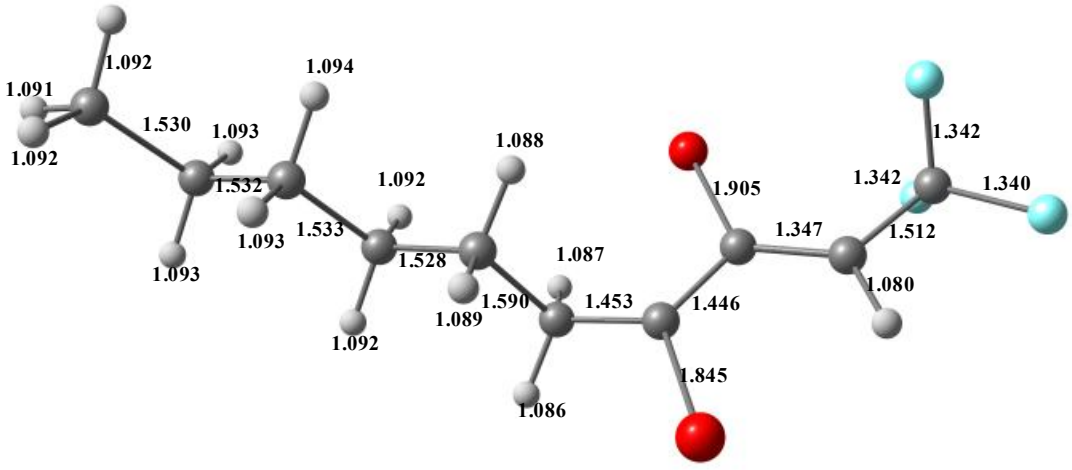
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.17252	1.99873	3.78933	0.03942	5.82748
Br	2	0.38792	27.99870	6.59829	0.01509	34.61208
C	3	-0.21368	1.99832	4.17770	0.03766	6.21368
Br	4	0.19323	27.99904	6.79276	0.01497	34.80677
C	5	-0.07402	1.99875	4.04978	0.02550	6.07402
C	6	1.05427	1.99933	2.89250	0.05390	4.94573
F	7	-0.34162	1.99991	7.33186	0.00985	9.34162
F	8	-0.33700	1.99991	7.32730	0.00979	9.33700
F	9	-0.33684	1.99991	7.32709	0.00983	9.33684
H	10	0.26654	0.00000	0.73051	0.00295	0.73346
C	11	-0.48794	1.99903	4.46414	0.02477	6.48794

H	12	0.26945	0.00000	0.72770	0.00285	0.73055
H	13	0.27094	0.00000	0.72662	0.00245	0.72906
C	14	-0.32391	1.99923	4.30753	0.01715	6.32391
H	15	0.21560	0.00000	0.78206	0.00234	0.78440
H	16	0.21593	0.00000	0.78168	0.00239	0.78407
C	17	-0.37806	1.99926	4.36033	0.01847	6.37806
H	18	0.20319	0.00000	0.79432	0.00248	0.79681
H	19	0.20422	0.00000	0.79334	0.00244	0.79578
C	20	-0.37351	1.99927	4.35660	0.01764	6.37351
H	21	0.19482	0.00000	0.80281	0.00236	0.80518
H	22	0.19507	0.00000	0.80258	0.00236	0.80493
C	23	-0.37815	1.99931	4.36257	0.01627	6.37815
H	24	0.19051	0.00000	0.80706	0.00243	0.80949
H	25	0.19062	0.00000	0.80696	0.00242	0.80938
C	26	-0.57000	1.99936	4.55999	0.01065	6.57000
H	27	0.19420	0.00000	0.80389	0.00191	0.80580
H	28	0.19419	0.00000	0.80390	0.00191	0.80581
H	29	0.20154	0.00000	0.79701	0.00145	0.79846

==========

* Total *	1.00000	81.98808	87.65823	0.35369	170.00000

Bond lengths, Å

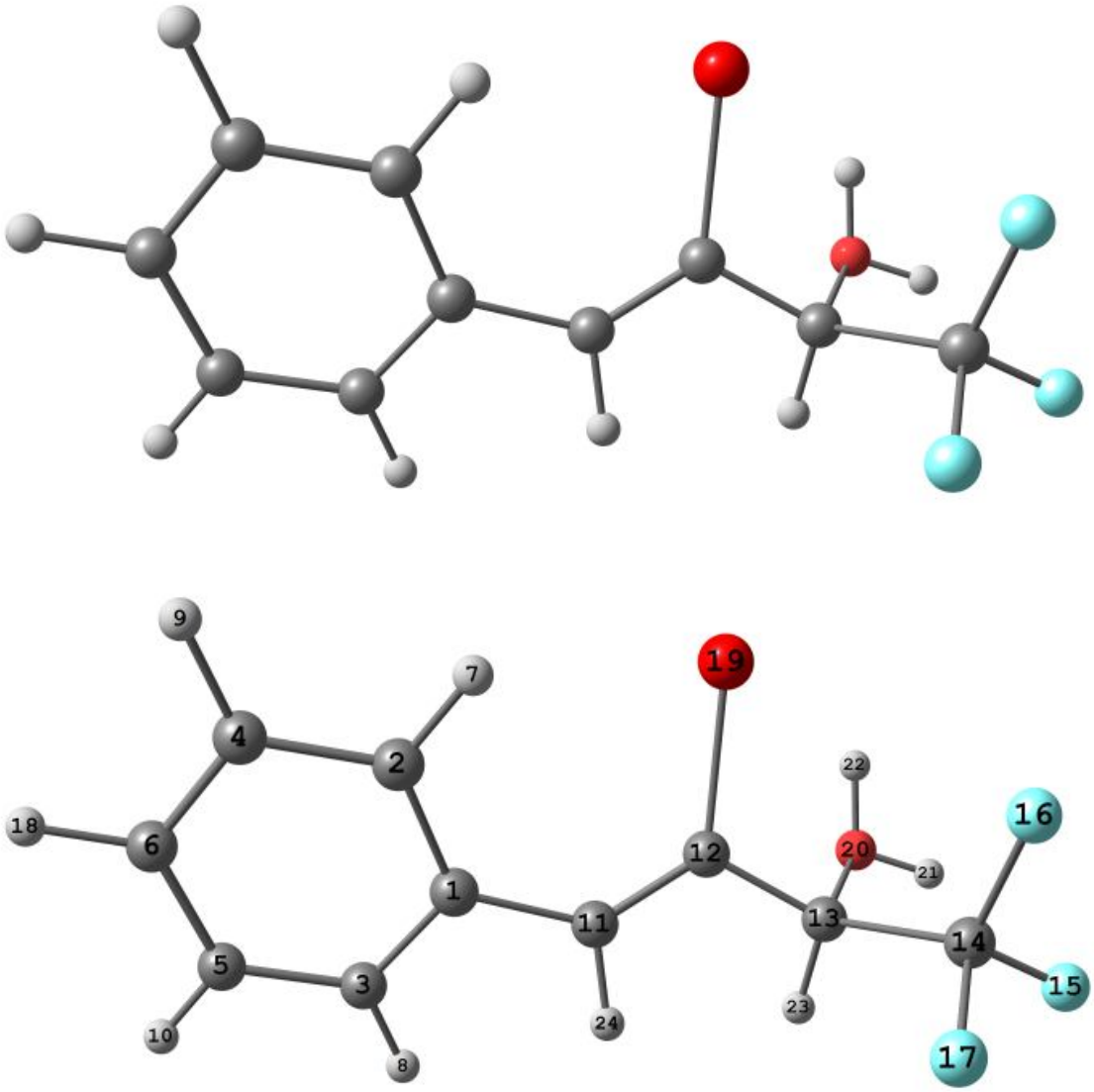


C1

E= -3335.38948886 h, G^{298}= -3335.259846 h μ= 8.78 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	2.139367	0.592702	-0.136444
2	C	2.631168	-0.533098	0.544942
3	C	3.058538	1.561219	-0.579290
4	C	3.994345	-0.686188	0.753510
5	C	4.420992	1.397200	-0.380497
6	C	4.893378	0.270053	0.286131
7	H	1.957578	-1.280082	0.929314
8	H	2.693875	2.443924	-1.086862
9	H	4.356736	-1.554539	1.285354
10	H	5.110899	2.148826	-0.736929
11	C	0.734515	0.863997	-0.411270
12	C	-0.378370	0.116780	-0.380765
13	C	-1.694847	0.738031	-0.664909
14	C	-2.678642	0.913784	0.511867
15	F	-3.870353	1.326955	0.032705
16	F	-2.889257	-0.199586	1.214819
17	F	-2.198359	1.853223	1.326690
18	H	5.954252	0.140774	0.448925
19	Br	-0.466273	-1.776430	-0.061874
20	O	-2.398646	-0.083077	-1.729274
21	H	-3.335917	0.156285	-1.872646
22	H	-2.307405	-1.048371	-1.551125
23	H	-1.575418	1.710285	-1.130376
24	H	0.553181	1.890349	-0.713463



Summary of Natural Population Analysis:

Natural Population

Natural ----------

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.11238	1.99898	4.09345	0.01995	6.11238
C	2	-0.16299	1.99907	4.14615	0.01777	6.16299
C	3	-0.15277	1.99909	4.13529	0.01840	6.15277
C	4	-0.20088	1.99916	4.18167	0.02005	6.20088
C	5	-0.20511	1.99915	4.18579	0.02018	6.20511
C	6	-0.17014	1.99915	4.15105	0.01994	6.17014
H	7	0.22128	0.00000	0.77671	0.00201	0.77872
H	8	0.21864	0.00000	0.77951	0.00185	0.78136

H	9	0.22020	0.00000	0.77813	0.00168	0.77980
H	10	0.22132	0.00000	0.77699	0.00170	0.77868
C	11	-0.11477	1.99883	4.09203	0.02391	6.11477
C	12	-0.19310	1.99853	4.16370	0.03087	6.19310
C	13	0.02847	1.99875	3.94239	0.03039	5.97153
C	14	1.06617	1.99928	2.87861	0.05594	4.93383
F	15	-0.35419	1.99992	7.34537	0.00890	9.35419
F	16	-0.33809	1.99991	7.32922	0.00895	9.33809
F	17	-0.33199	1.99991	7.32314	0.00894	9.33199
H	18	0.21910	0.00000	0.77936	0.00154	0.78090
Br	19	0.11408	27.99903	6.87020	0.01669	34.88592
O	20	-0.63488	1.99973	6.61576	0.01939	8.63488
H	21	0.57890	0.00000	0.41851	0.00260	0.42110
H	22	0.56820	0.00000	0.42774	0.00406	0.43180
H	23	0.27665	0.00000	0.72038	0.00296	0.72335
H	24	0.23829	0.00000	0.75961	0.00211	0.76171

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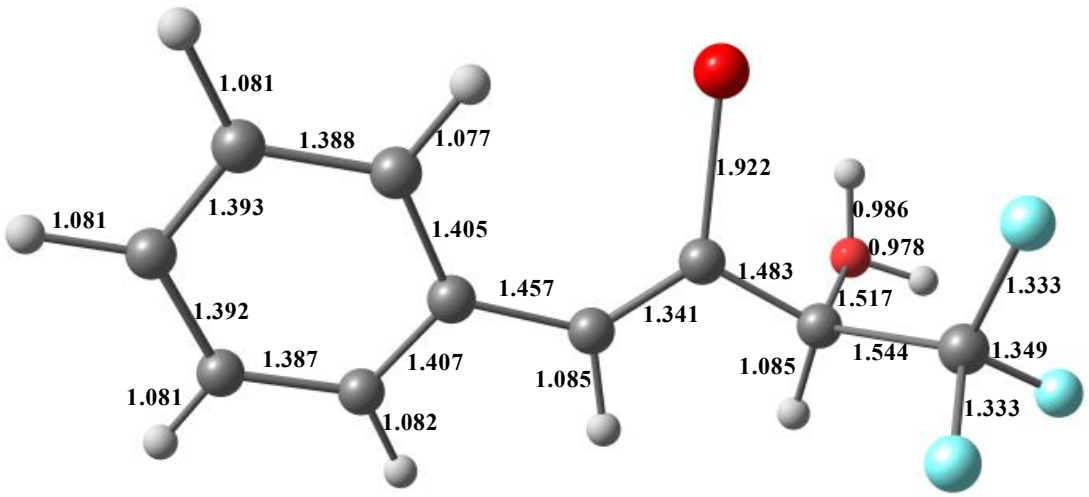
* Total *	1.00000	55.98848	81.67077	0.34075	138.00000

Bond lengths, Å

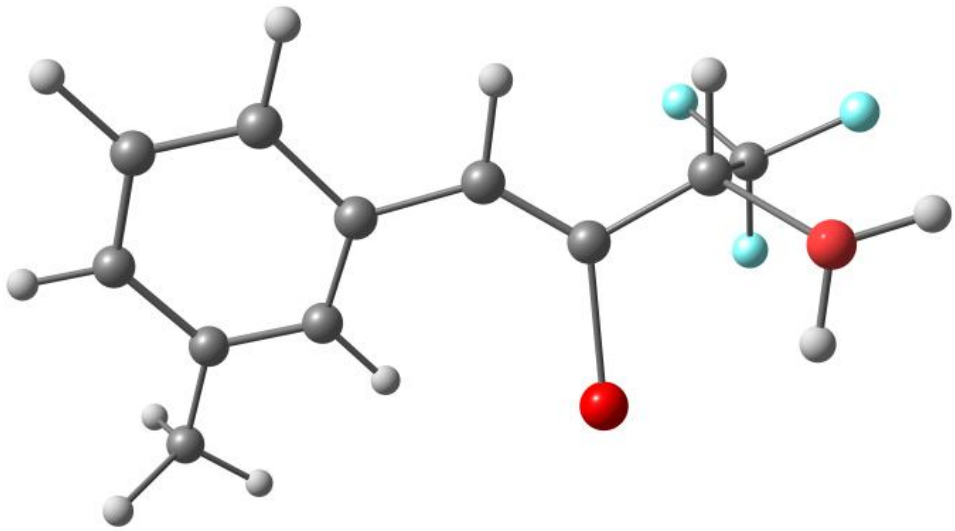


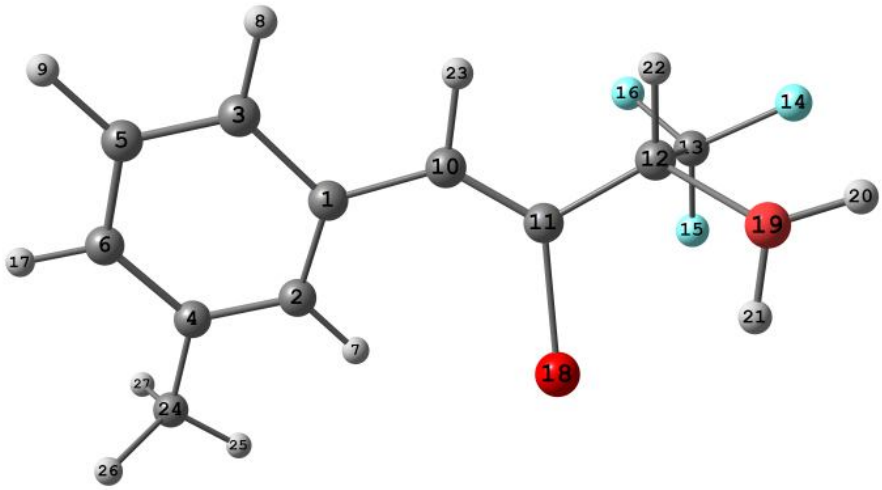
C2

E= -3374.71931665 h, G^{298}= -3374.56549 h μ= 9.27 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	-1.813189	-0.897040	-0.218007
2	C	-2.453649	0.271548	0.230900
3	C	-2.600699	-2.023895	-0.507693
4	C	-3.835878	0.333478	0.372884
5	C	-3.980349	-1.970771	-0.375362
6	C	-4.593034	-0.801755	0.058942
7	H	-1.874361	1.142811	0.486333
8	H	-2.125047	-2.936861	-0.838711
9	H	-4.577460	-2.841867	-0.605574
10	C	-0.377836	-1.054441	-0.404849
11	C	0.666854	-0.212558	-0.400319
12	C	2.041276	-0.739739	-0.577505
13	C	2.986247	-0.720784	0.640839
14	F	4.219509	-1.102499	0.248638
15	F	3.098106	0.472985	1.225071
16	F	2.534298	-1.597492	1.537745
17	H	-5.669857	-0.768833	0.162978
18	Br	0.589683	1.702842	-0.250096
19	O	2.716341	0.043141	-1.691467
20	H	3.681322	-0.095057	-1.769805
21	H	2.503230	1.003543	-1.623831
22	H	2.024203	-1.757279	-0.953042
23	H	-0.090821	-2.083487	-0.594804
24	C	-4.511142	1.594763	0.848487
25	H	-3.783353	2.358503	1.115440
26	H	-5.160075	2.004182	0.072391
27	H	-5.136253	1.399957	1.720721





Summary of Natural Population Analysis:

Natural Population

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.10641	1.99898	4.08775	0.01967	6.10641
C	2	-0.16875	1.99896	4.15262	0.01717	6.16875
C	3	-0.16017	1.99909	4.14293	0.01816	6.16017
C	4	-0.02368	1.99905	4.00748	0.01715	6.02368
C	5	-0.19892	1.99915	4.17965	0.02013	6.19892
C	6	-0.16778	1.99905	4.14978	0.01896	6.16778
H	7	0.21763	0.00000	0.78001	0.00236	0.78237
H	8	0.21764	0.00000	0.78056	0.00180	0.78236

H	9	0.22024	0.00000	0.77794	0.00181	0.77976
C	10	-0.11313	1.99884	4.09029	0.02400	6.11313
C	11	-0.19610	1.99853	4.16695	0.03062	6.19610
C	12	0.02853	1.99875	3.94234	0.03037	5.97147
C	13	1.06568	1.99927	2.87913	0.05592	4.93432
F	14	-0.35407	1.99992	7.34526	0.00890	9.35407
F	15	-0.33838	1.99991	7.32953	0.00894	9.33838
F	16	-0.33216	1.99991	7.32333	0.00893	9.33216
H	17	0.21611	0.00000	0.78218	0.00171	0.78389
Br	18	0.11367	27.99903	6.87061	0.01669	34.88633
O	19	-0.63696	1.99973	6.61789	0.01934	8.63696
H	20	0.57853	0.00000	0.41885	0.00262	0.42147
H	21	0.56715	0.00000	0.42871	0.00414	0.43285
H	22	0.27642	0.00000	0.72061	0.00297	0.72358
H	23	0.23698	0.00000	0.76093	0.00209	0.76302
C	24	-0.59133	1.99929	4.58024	0.01180	6.59133
H	25	0.21184	0.00000	0.78677	0.00139	0.78816
H	26	0.21924	0.00000	0.77927	0.00149	0.78076
H	27	0.21817	0.00000	0.78035	0.00148	0.78183

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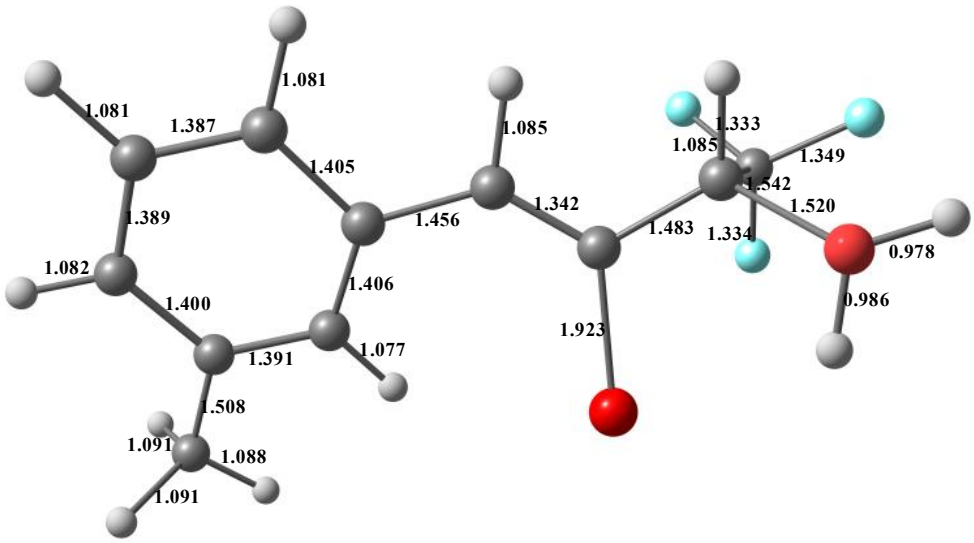
* Total *	1.00000	57.98743	87.66196	0.35061	146.00000

Bond lengths, Å

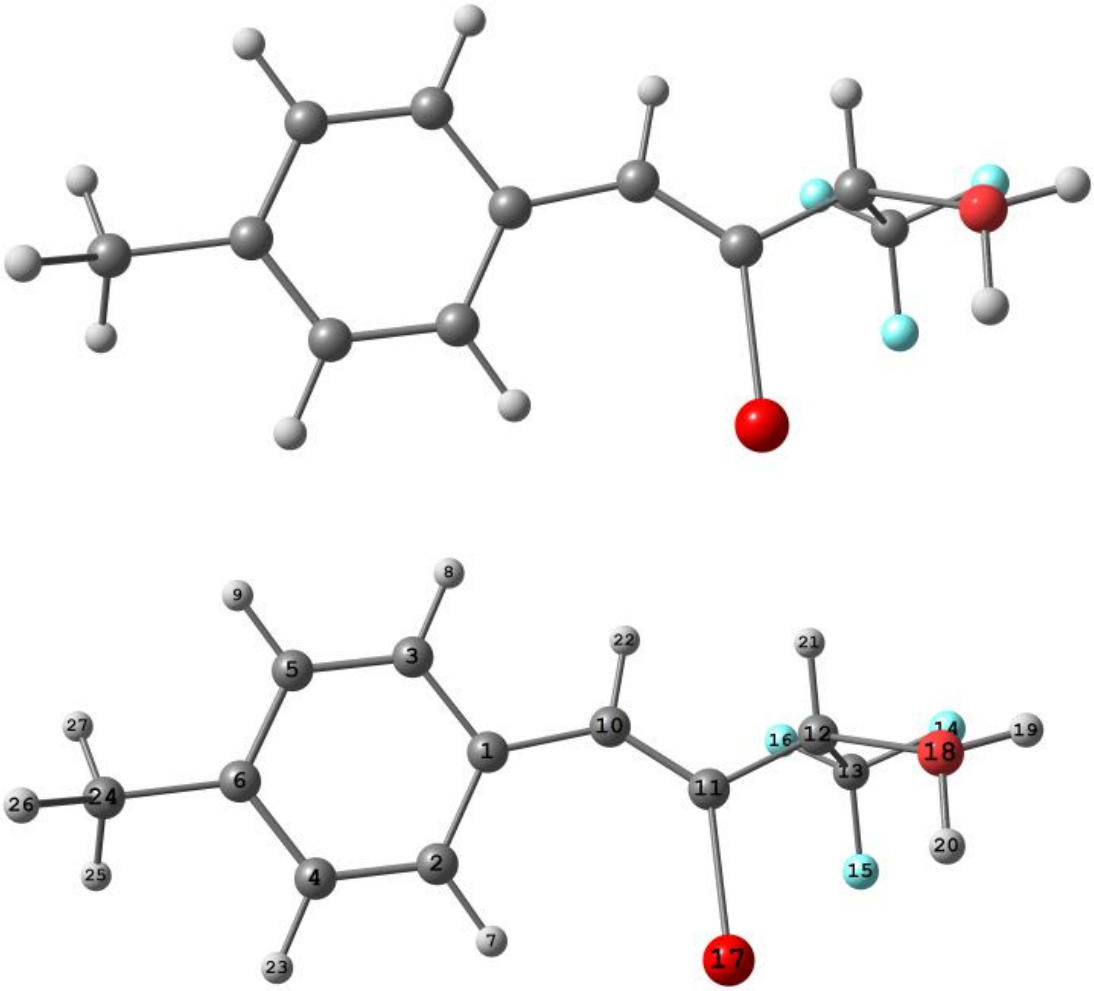


C3

E= -3374.72047496 h, G^{298}= -3374.566727 h μ= 9.15 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.786305	-0.573532	0.205153
2	C	2.312700	0.595521	-0.371478
3	C	2.691545	-1.584791	0.576209
4	C	3.678902	0.740776	-0.546409
5	C	4.056480	-1.426233	0.405646
6	C	4.578839	-0.257168	-0.154683
7	H	1.662138	1.387897	-0.700141
8	H	2.312703	-2.502954	1.004795
9	H	4.725716	-2.221983	0.704051
10	C	0.379519	-0.847756	0.442565
11	C	-0.743563	-0.113573	0.379152
12	C	-2.054441	-0.746975	0.644911
13	C	-3.038309	-0.917637	-0.531937
14	F	-4.223544	-1.354209	-0.055679
15	F	-3.267266	0.201686	-1.219491
16	F	-2.548186	-1.839406	-1.361309
17	Br	-0.848117	1.775895	0.039191
18	O	-2.774068	0.057741	1.720977
19	H	-3.710929	-0.189223	1.852804
20	H	-2.690482	1.024819	1.554085
21	H	-1.931281	-1.722933	1.101210
22	H	0.197345	-1.875677	0.739317
23	H	4.056678	1.646953	-1.001010
24	C	6.062043	-0.068338	-0.318009
25	H	6.290866	0.531258	-1.197992
26	H	6.477793	0.453048	0.547667
27	H	6.576934	-1.023878	-0.402688



Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.12742	1.99899	4.10887	0.01957	6.12742
C	2	-0.15370	1.99907	4.13722	0.01741	6.15370
C	3	-0.14174	1.99909	4.12455	0.01810	6.14174
C	4	-0.20365	1.99904	4.18536	0.01924	6.20365
C	5	-0.20994	1.99903	4.19154	0.01937	6.20994
C	6	0.01369	1.99905	3.96980	0.01746	5.98631
H	7	0.22085	0.00000	0.77706	0.00209	0.77915
H	8	0.21744	0.00000	0.78070	0.00186	0.78256

H	9	0.21863	0.00000	0.77940	0.00197	0.78137
C	10	-0.10164	1.99872	4.07930	0.02363	6.10164
C	11	-0.20625	1.99855	4.17679	0.03090	6.20625
C	12	0.02812	1.99874	3.94292	0.03021	5.97188
C	13	1.06593	1.99927	2.87890	0.05590	4.93407
F	14	-0.35509	1.99992	7.34627	0.00890	9.35509
F	15	-0.33821	1.99991	7.32935	0.00896	9.33821
F	16	-0.33238	1.99991	7.32355	0.00892	9.33238
Br	17	0.10826	27.99903	6.87576	0.01695	34.89174
O	18	-0.63693	1.99973	6.61780	0.01940	8.63693
H	19	0.57753	0.00000	0.41984	0.00263	0.42247
H	20	0.56802	0.00000	0.42802	0.00396	0.43198
H	21	0.27571	0.00000	0.72134	0.00295	0.72429
H	22	0.23533	0.00000	0.76252	0.00215	0.76467
H	23	0.21736	0.00000	0.78072	0.00192	0.78264
C	24	-0.59734	1.99928	4.58596	0.01210	6.59734
H	25	0.21691	0.00000	0.78155	0.00154	0.78309
H	26	0.22481	0.00000	0.77361	0.00158	0.77519
H	27	0.21570	0.00000	0.78276	0.00154	0.78430

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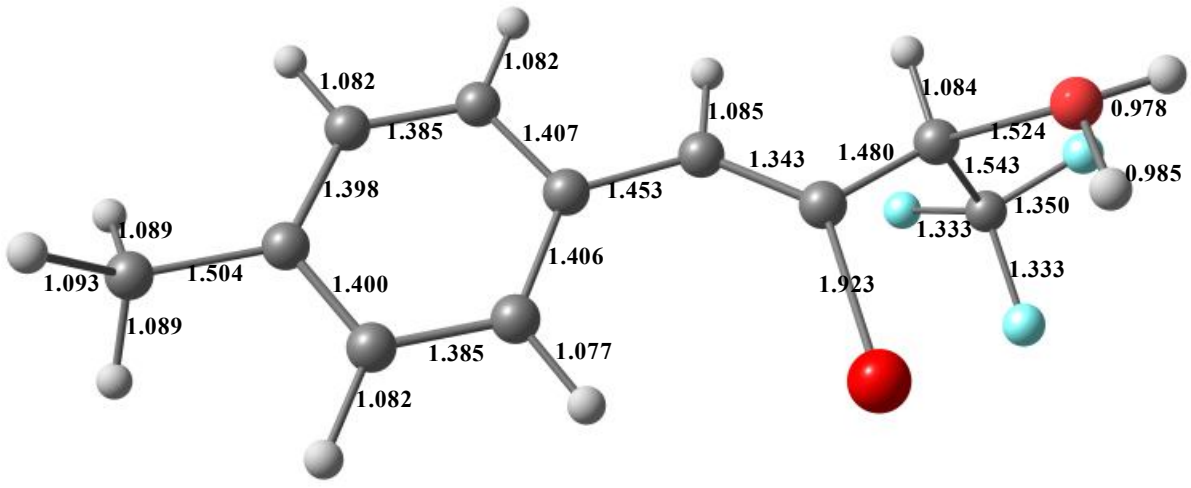
* Total *	1.00000	57.98733	87.66146	0.35121	146.00000

Bond lengths, Å

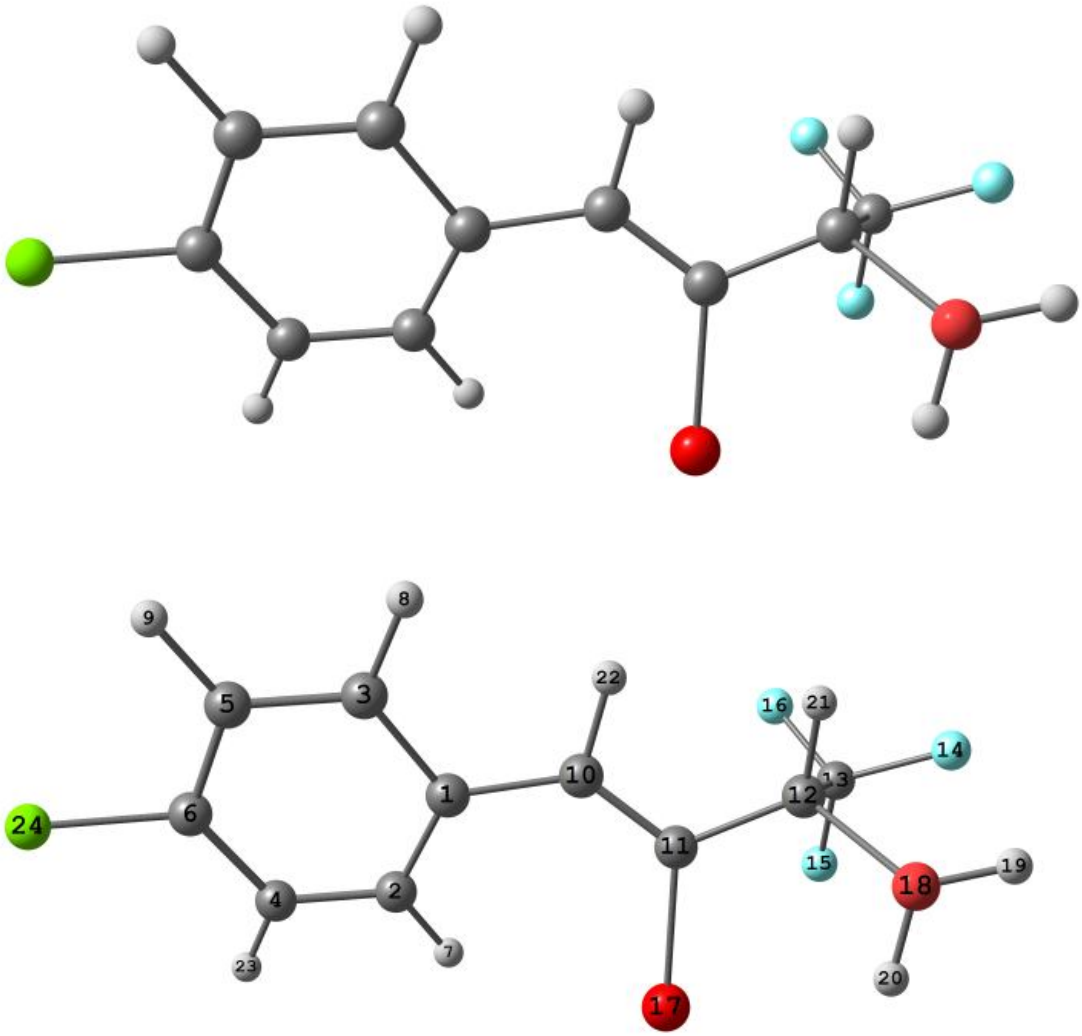


C4

E= -3795.01356929 h, G^{298}= -3794.895654 h μ= 13.32 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.454261	-0.577813	0.233189
2	C	1.976864	0.580648	-0.364754
3	C	2.356698	-1.572476	0.650252
4	C	3.344009	0.744346	-0.521108
5	C	3.725191	-1.414366	0.507681
6	C	4.207034	-0.250466	-0.076851
7	H	1.326177	1.357995	-0.726257
8	H	1.978752	-2.481077	1.097895
9	H	4.404826	-2.183772	0.840252
10	C	0.042113	-0.855142	0.453486
11	C	-1.073866	-0.114413	0.384818
12	C	-2.393426	-0.743148	0.637860
13	C	-3.356667	-0.918766	-0.555762
14	F	-4.552180	-1.342941	-0.095628
15	F	-3.565427	0.196547	-1.255973
16	F	-2.857374	-1.850383	-1.367789
17	Br	-1.166305	1.775668	0.056044
18	O	-3.119969	0.069564	1.693611
19	H	-4.058301	-0.175824	1.818887
20	H	-3.031491	1.036309	1.523807
21	H	-2.278920	-1.716958	1.101205
22	H	-0.144125	-1.883751	0.743756
23	H	3.734767	1.636558	-0.985838
24	Cl	5.937077	-0.034930	-0.267205



Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.11057	1.99898	4.09210	0.01948	6.11057
C	2	-0.14322	1.99906	4.12688	0.01728	6.14322
C	3	-0.13297	1.99908	4.11601	0.01787	6.13297
C	4	-0.22212	1.99896	4.20107	0.02209	6.22212
C	5	-0.22674	1.99895	4.20559	0.02220	6.22674
C	6	-0.01687	1.99855	3.99073	0.02759	6.01687
H	7	0.22787	0.00000	0.77010	0.00203	0.77213
H	8	0.22542	0.00000	0.77273	0.00185	0.77458
H	9	0.23713	0.00000	0.76072	0.00215	0.76287

C	10	-0.11723	1.99884	4.09464	0.02376	6.11723
C	11	-0.19083	1.99853	4.16139	0.03091	6.19083
C	12	0.02856	1.99875	3.94230	0.03038	5.97144
C	13	1.06632	1.99928	2.87844	0.05596	4.93368
F	14	-0.35412	1.99992	7.34531	0.00889	9.35412
F	15	-0.33774	1.99991	7.32888	0.00895	9.33774
F	16	-0.33157	1.99991	7.32274	0.00893	9.33157
Br	17	0.11749	27.99903	6.86680	0.01668	34.88251
O	18	-0.63450	1.99973	6.61542	0.01934	8.63450
H	19	0.57908	0.00000	0.41832	0.00260	0.42092
H	20	0.56873	0.00000	0.42728	0.00399	0.43127
H	21	0.27680	0.00000	0.72025	0.00296	0.72320
H	22	0.23925	0.00000	0.75864	0.00211	0.76075
H	23	0.23592	0.00000	0.76198	0.00210	0.76408
Cl	24	0.01590	9.99959	6.96642	0.01809	16.98410

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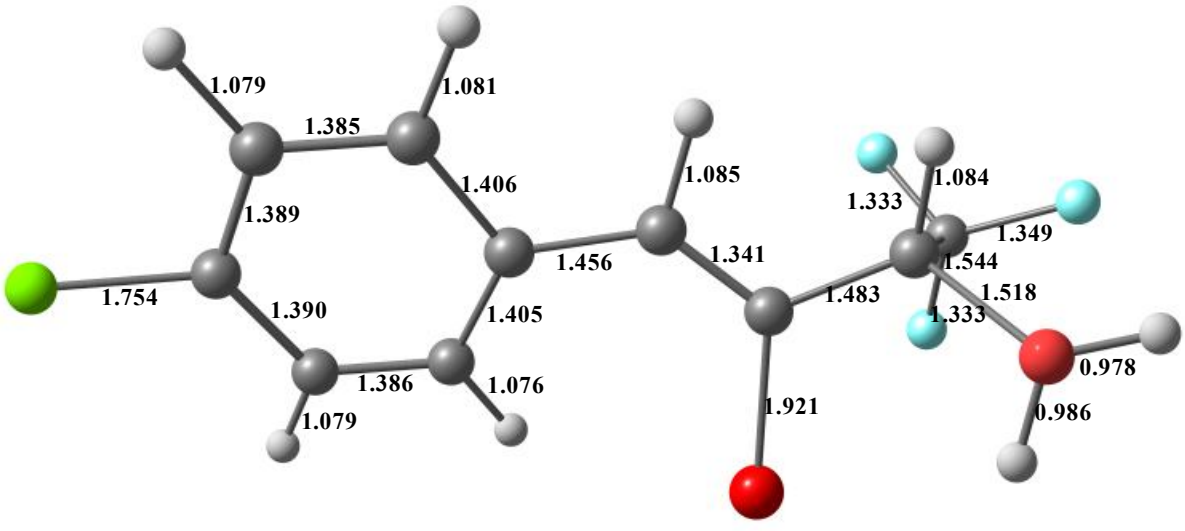
* Total *	1.00000	65.98706	87.64473	0.36821	154.00000

Bond lengths, Å

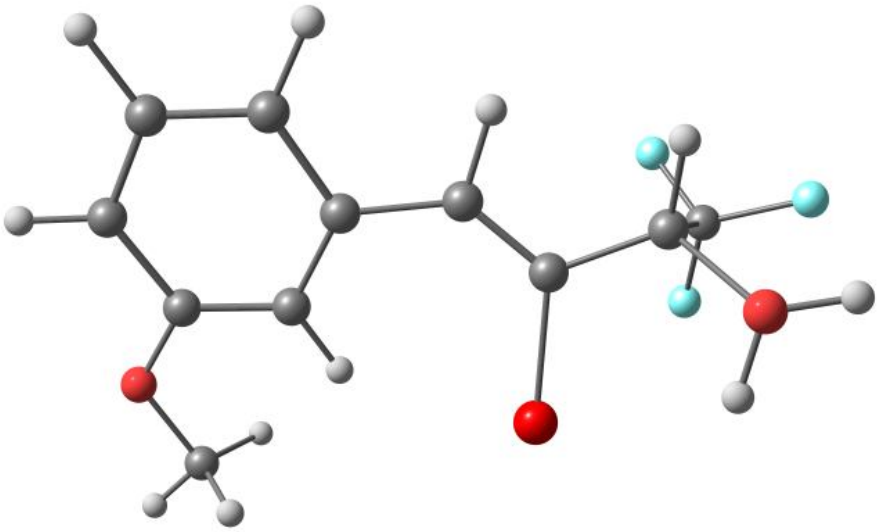


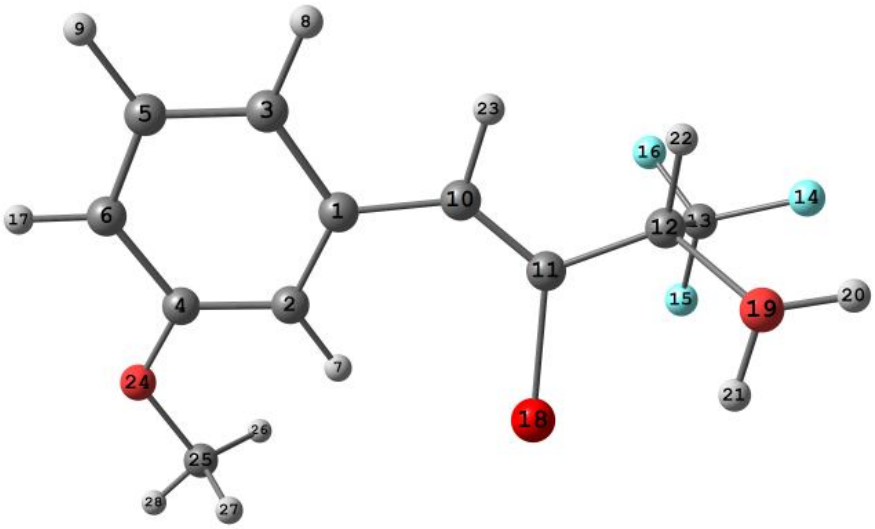
C5

E= -3449.95176444 h, G^{298}= -3449.792642 h μ= 11.34 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.537718	1.164138	-0.227765
2	C	2.273012	0.008058	0.093951
3	C	2.216505	2.377683	-0.412595
4	C	3.657177	0.075370	0.212367
5	C	3.600692	2.431699	-0.297147
6	C	4.322882	1.291917	0.012158
7	H	1.768439	-0.925184	0.258845
8	H	1.659257	3.273099	-0.648247
9	H	4.117596	3.368986	-0.445906
10	C	0.090001	1.216270	-0.381854
11	C	-0.886759	0.297201	-0.415696
12	C	-2.301918	0.727615	-0.530408
13	C	-3.207982	0.572258	0.709311
14	F	-4.485351	0.827911	0.356660
15	F	-3.175912	-0.641213	1.260678
16	F	-2.830037	1.468602	1.621003
17	H	5.399026	1.319942	0.107716
18	Br	-0.663351	-1.612143	-0.393213
19	O	-2.949403	-0.039039	-1.667968
20	H	-3.921977	0.050305	-1.718073
21	H	-2.682901	-0.987996	-1.650509
22	H	-2.370822	1.762818	-0.847264
23	H	-0.278894	2.230250	-0.494579
24	O	4.449929	-0.985209	0.520253
25	C	3.837664	-2.261688	0.722221
26	H	3.145370	-2.235980	1.564470
27	H	3.315189	-2.592135	-0.176308
28	H	4.650540	-2.945964	0.941696





Summary of Natural Population Analysis:

Natural Population

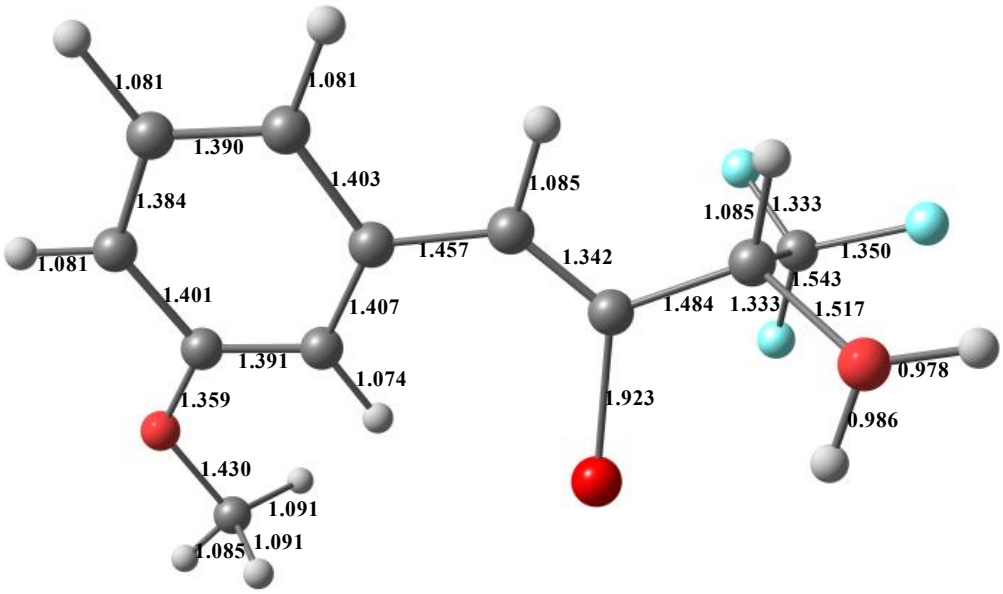
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.09166	1.99900	4.07306	0.01960	6.09166
C	2	-0.25608	1.99896	4.24085	0.01627	6.25608
C	3	-0.17958	1.99908	4.16198	0.01852	6.17958
C	4	0.33026	1.99880	3.64936	0.02158	5.66974
C	5	-0.19039	1.99916	4.17163	0.01959	6.19039
C	6	-0.20833	1.99906	4.18907	0.02020	6.20833
H	7	0.22862	0.00000	0.76877	0.00261	0.77138

H	8	0.21897	0.00000	0.77926	0.00177	0.78103
H	9	0.22245	0.00000	0.77582	0.00173	0.77755
C	10	-0.11588	1.99884	4.09306	0.02397	6.11588
C	11	-0.19401	1.99853	4.16493	0.03055	6.19401
C	12	0.02824	1.99875	3.94267	0.03034	5.97176
C	13	1.06610	1.99928	2.87873	0.05590	4.93390
F	14	-0.35456	1.99992	7.34576	0.00889	9.35456
F	15	-0.33785	1.99991	7.32901	0.00893	9.33785
F	16	-0.33223	1.99991	7.32339	0.00893	9.33223
H	17	0.22698	0.00000	0.77102	0.00200	0.77302
Br	18	0.11537	27.99903	6.86878	0.01682	34.88463
O	19	-0.63524	1.99973	6.61613	0.01937	8.63524
H	20	0.57884	0.00000	0.41855	0.00261	0.42116
H	21	0.56764	0.00000	0.42829	0.00407	0.43236
H	22	0.27671	0.00000	0.72034	0.00295	0.72329
H	23	0.23798	0.00000	0.75998	0.00204	0.76202
O	24	-0.55144	1.99971	6.52730	0.02443	8.55144
C	25	-0.20973	1.99923	4.19696	0.01354	6.20973
H	26	0.18003	0.00000	0.81777	0.00220	0.81997
H	27	0.18018	0.00000	0.81759	0.00224	0.81982
H	28	0.19861	0.00000	0.80016	0.00123	0.80139

==========

* Total *	1.00000	59.98687	93.63022	0.38291	154.00000

Bond lengths, Å

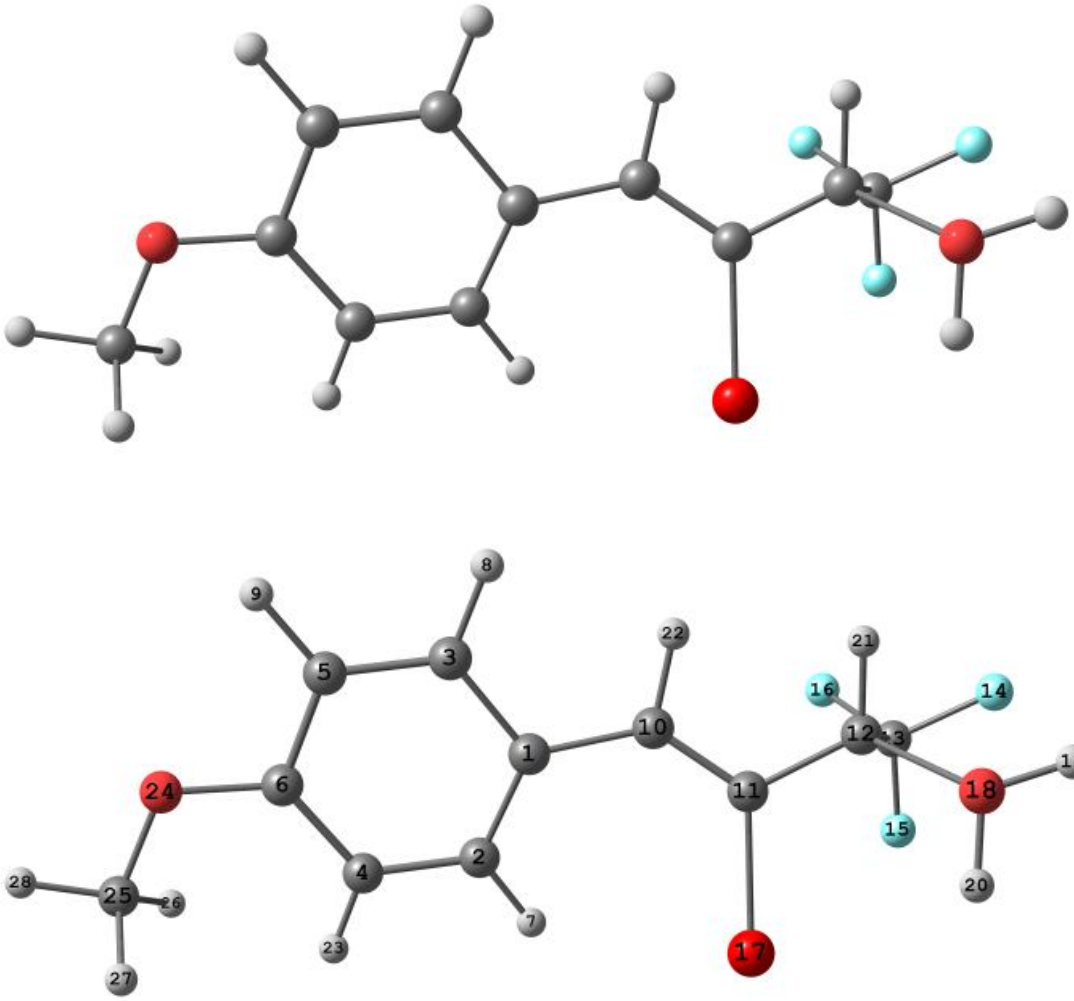


C6

E= -3449.95512611 h, G^{298}= -3449.79603 h μ= 9.31 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.437484	-0.711039	0.243352
2	C	2.027649	0.476827	-0.219831
3	C	2.299172	-1.785022	0.559232
4	C	3.401359	0.597856	-0.350559
5	C	3.666326	-1.673321	0.443941
6	C	4.234473	-0.475389	-0.012188
7	H	1.417532	1.319244	-0.497291
8	H	1.875164	-2.717795	0.905536
9	H	4.315798	-2.499303	0.695183
10	C	0.020701	-0.948519	0.413278
11	C	-1.080860	-0.174610	0.356876
12	C	-2.410001	-0.781723	0.537828
13	C	-3.415374	-0.749797	-0.630778
14	F	-4.586436	-1.281279	-0.222008
15	F	-3.672281	0.471587	-1.102179
16	F	-2.932278	-1.501460	-1.621197
17	Br	-1.104202	1.737015	0.151364
18	O	-3.099725	-0.104336	1.737730
19	H	-4.029286	-0.368550	1.884375
20	H	-3.021411	0.873086	1.693023
21	H	-2.328762	-1.815000	0.857461
22	H	-0.205019	-1.986731	0.634372
23	H	3.812948	1.524754	-0.716349
24	O	5.580978	-0.454047	-0.096980
25	C	6.228049	0.736986	-0.564163
26	H	5.920582	0.971663	-1.582906
27	H	6.014422	1.578954	0.093791
28	H	7.290157	0.518073	-0.544408



Summary of Natural Population Analysis:

Natural Population

Natural ----------

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.14648	1.99898	4.12792	0.01958	6.14648
C	2	-0.13317	1.99909	4.11648	0.01761	6.13317
C	3	-0.13310	1.99910	4.11632	0.01768	6.13310
C	4	-0.28310	1.99905	4.26610	0.01795	6.28310
C	5	-0.24892	1.99905	4.22926	0.02061	6.24892
C	6	0.36678	1.99882	3.61242	0.02199	5.63322
H	7	0.22329	0.00000	0.77463	0.00207	0.77671
H	8	0.21975	0.00000	0.77841	0.00184	0.78025
H	9	0.22992	0.00000	0.76791	0.00217	0.77008
C	10	-0.10457	1.99886	4.08197	0.02374	6.10457

C	11	-0.21365	1.99852	4.18444	0.03069	6.21365
C	12	0.02627	1.99873	3.94450	0.03050	5.97373
C	13	1.06556	1.99926	2.87926	0.05592	4.93444
F	14	-0.35501	1.99992	7.34618	0.00892	9.35501
F	15	-0.33927	1.99991	7.33036	0.00900	9.33927
F	16	-0.33284	1.99991	7.32407	0.00886	9.33284
Br	17	0.09849	27.99905	6.88561	0.01685	34.90151
O	18	-0.64333	1.99974	6.62443	0.01917	8.64333
H	19	0.57622	0.00000	0.42114	0.00264	0.42378
H	20	0.56927	0.00000	0.42719	0.00354	0.43073
H	21	0.27494	0.00000	0.72207	0.00298	0.72506
H	22	0.23429	0.00000	0.76358	0.00213	0.76571
H	23	0.22991	0.00000	0.76798	0.00211	0.77009
O	24	-0.53757	1.99970	6.51266	0.02521	8.53757
C	25	-0.21000	1.99922	4.19737	0.01340	6.21000
H	26	0.18317	0.00000	0.81466	0.00216	0.81683
H	27	0.18330	0.00000	0.81454	0.00217	0.81670
H	28	0.19986	0.00000	0.79890	0.00123	0.80014

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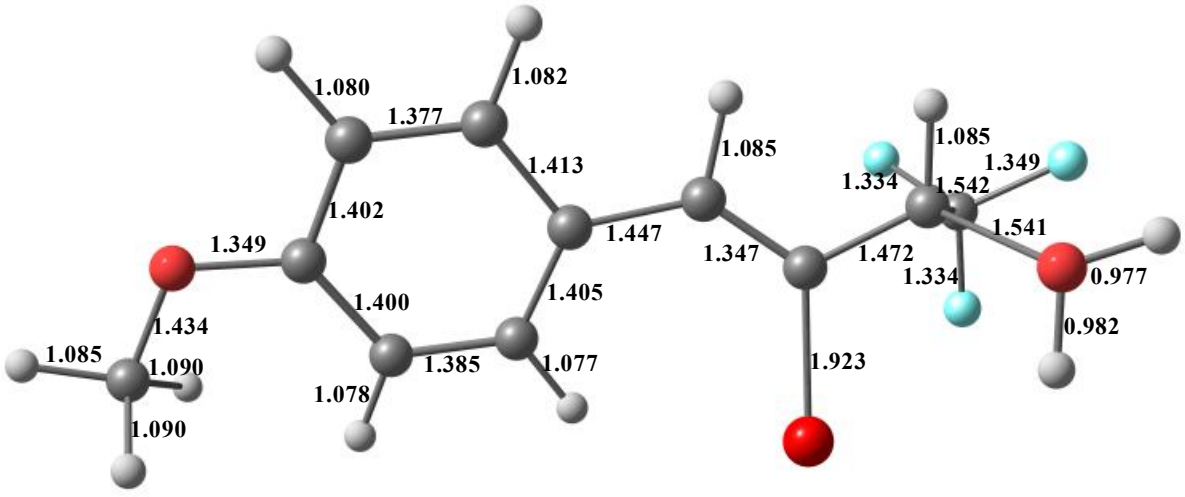
* Total *	1.00000	59.98689	93.63038	0.38273	154.00000

Bond lengths, Å



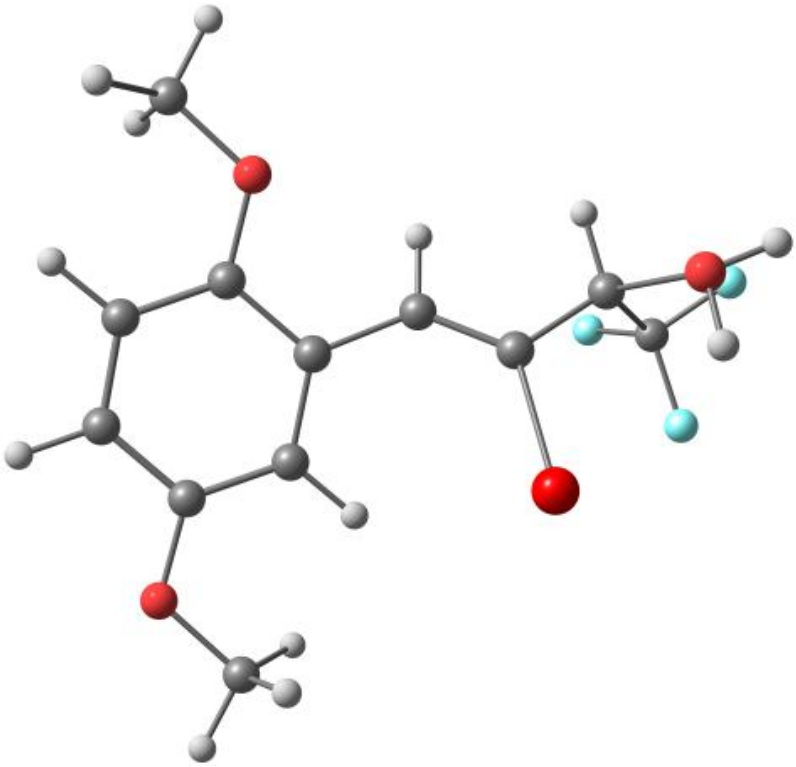
C7

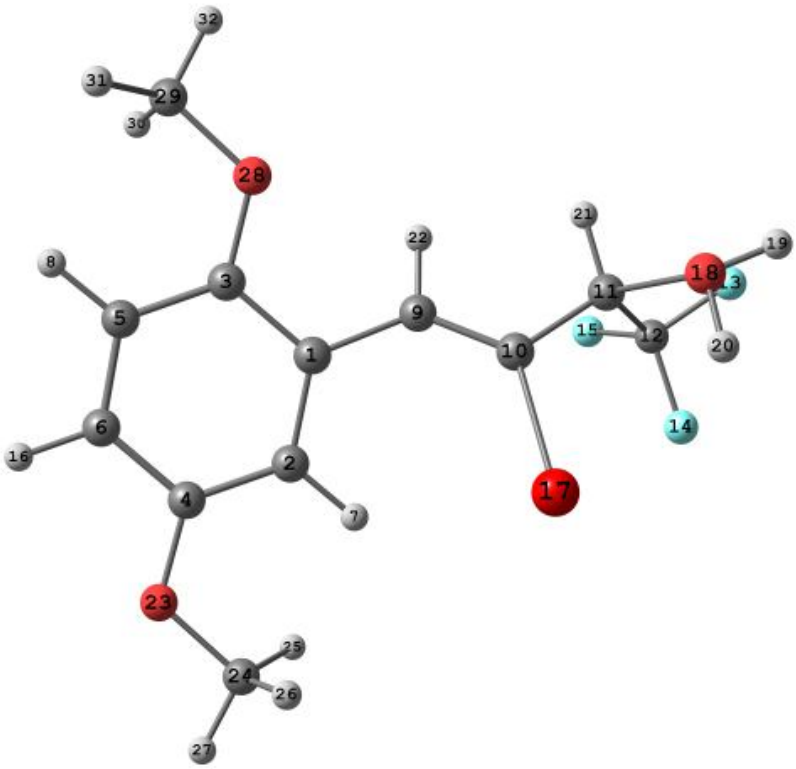
E= -3564.51190533 h, G^{298}= -3564.32455 h μ= 11.01 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.473429	0.547571	0.049612
2	C	1.902720	-0.771688	0.283061
3	C	2.438352	1.572850	-0.075727
4	C	3.253055	-1.071749	0.385293
5	C	3.795167	1.257862	0.020895
6	C	4.194627	-0.047788	0.247027
7	H	1.166818	-1.543841	0.419516
8	H	4.545971	2.024849	-0.080031
9	C	0.076654	0.939347	0.000241
10	C	-1.044597	0.269845	-0.306192
11	C	-2.363355	0.925290	-0.161880
12	C	-3.298992	0.435002	0.961768
13	F	-4.493265	1.051487	0.841741
14	F	-3.520372	-0.880542	0.948414
15	F	-2.763160	0.769310	2.135809
16	H	5.245491	-0.288510	0.324452
17	Br	-1.128815	-1.511266	-1.031191
18	O	-3.122505	0.786442	-1.473111
19	H	-4.061682	1.055476	-1.433795
20	H	-3.031134	-0.122963	-1.841092
21	H	-2.253166	1.997995	-0.043529
22	H	-0.089629	1.979148	0.258285
23	O	3.756302	-2.318083	0.624966
24	C	2.835756	-3.399327	0.773718
25	H	2.179579	-3.243044	1.631392
26	H	2.236355	-3.532493	-0.128221
27	H	3.442125	-4.283972	0.939351
28	O	1.968822	2.826072	-0.308657
29	C	2.897360	3.914705	-0.340663
30	H	3.447092	3.987248	0.597813
31	H	3.593688	3.808489	-1.172441

32 H 2.296191 4.806659 -0.482194





Summary of Natural Population Analysis:

Natural Population

Natural ----------

Atom No Charge Core Valence Rydberg Total

C	1	-0.13501	1.99894	4.11653	0.01954	6.13501
C	2	-0.23661	1.99897	4.22172	0.01591	6.23661
C	3	0.35766	1.99874	3.62316	0.02044	5.64234
C	4	0.29935	1.99876	3.68044	0.02145	5.70065
C	5	-0.26751	1.99906	4.25103	0.01742	6.26751
C	6	-0.18796	1.99908	4.16894	0.01994	6.18796
H	7	0.22914	0.00000	0.76838	0.00248	0.77086
H	8	0.23066	0.00000	0.76718	0.00215	0.76934
C	9	-0.11498	1.99882	4.09138	0.02478	6.11498
C	10	-0.19733	1.99853	4.16779	0.03102	6.19733
C	11	0.02735	1.99874	3.94344	0.03047	5.97265
C	12	1.06562	1.99927	2.87922	0.05589	4.93438
F	13	-0.35461	1.99992	7.34579	0.00890	9.35461
F	14	-0.33885	1.99991	7.32997	0.00897	9.33885
F	15	-0.33212	1.99991	7.32326	0.00896	9.33212
H	16	0.22718	0.00000	0.77077	0.00204	0.77282
Br	17	0.10402	27.99904	6.87993	0.01701	34.89598
O	18	-0.63727	1.99973	6.61824	0.01930	8.63727
H	19	0.57819	0.00000	0.41920	0.00261	0.42181
H	20	0.56827	0.00000	0.42770	0.00403	0.43173
H	21	0.27655	0.00000	0.72045	0.00300	0.72345
H	22	0.24898	0.00000	0.74818	0.00284	0.75102
O	23	-0.55703	1.99971	6.53296	0.02435	8.55703
C	24	-0.20890	1.99924	4.19585	0.01381	6.20890
H	25	0.17772	0.00000	0.81999	0.00229	0.82228
H	26	0.17790	0.00000	0.81975	0.00235	0.82210
H	27	0.19719	0.00000	0.80157	0.00125	0.80281
O	28	-0.55251	1.99970	6.53032	0.02249	8.55251
C	29	-0.20683	1.99923	4.19386	0.01374	6.20683
H	30	0.18154	0.00000	0.81612	0.00234	0.81846
H	31	0.18129	0.00000	0.81647	0.00224	0.81871
H	32	0.19891	0.00000	0.79983	0.00127	0.80109

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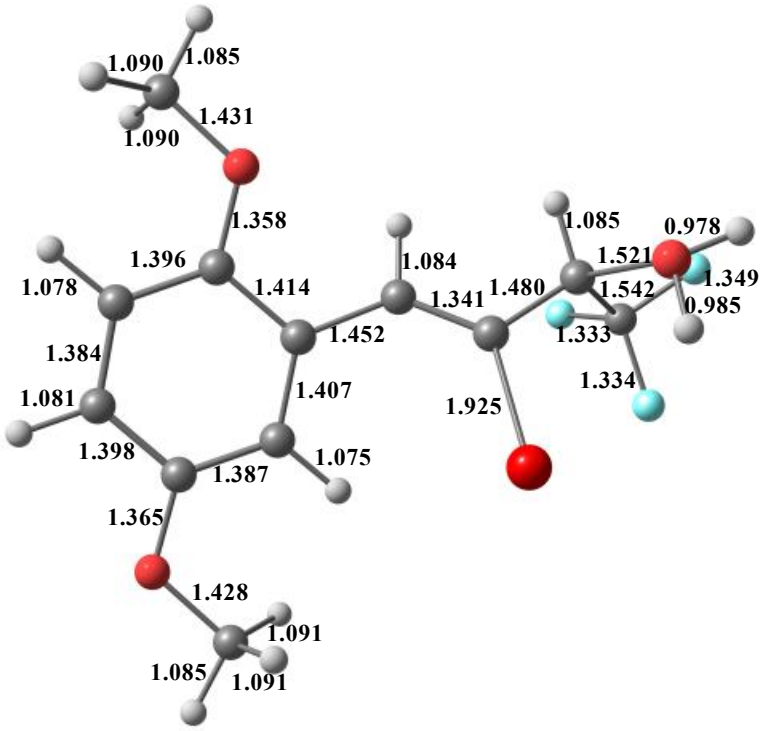
* Total *	1.00000	63.98528	105.58944	0.42528	170.00000

Bond lengths, Å

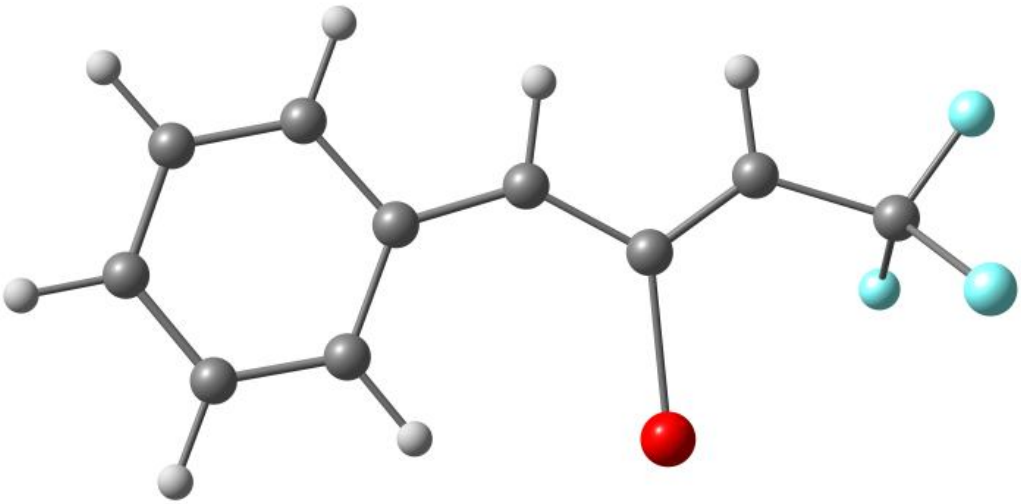


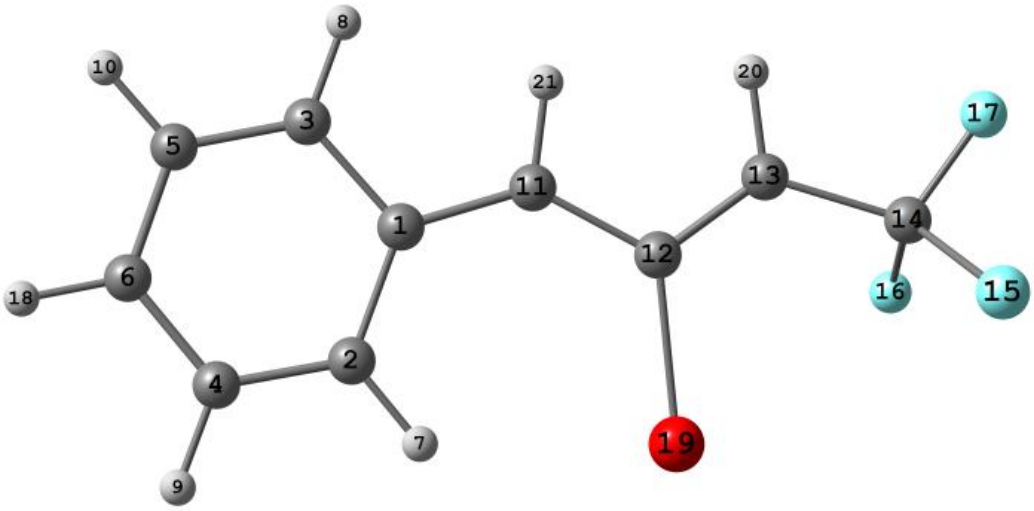
D1

E= -3258.92590446 h, G^{298}= -3258.824059 h μ= 12.42 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	2.102084	0.610472	0.000002
2	C	2.572984	-0.740317	0.000615
3	C	3.069061	1.670995	-0.000690
4	C	3.921612	-0.994684	0.000488
5	C	4.414026	1.397051	-0.000876
6	C	4.840381	0.064861	-0.000280
7	H	1.875990	-1.558305	0.001256
8	H	2.721438	2.693991	-0.001138
9	H	4.278939	-2.013206	0.000989
10	H	5.136399	2.198914	-0.001445
11	C	0.773262	1.023436	0.000005
12	C	-0.497356	0.354617	0.000091
13	C	-1.581784	1.159402	0.000070
14	C	-3.029708	0.735343	0.000062
15	F	-3.342815	0.009160	-1.086864
16	F	-3.342839	0.009159	1.086994
17	F	-3.816394	1.823779	0.000057
18	H	5.899151	-0.153687	-0.000389
19	Br	-0.688761	-1.536117	0.000064
20	H	-1.444524	2.231207	0.000058
21	H	0.650297	2.099235	-0.000174





Summary of Natural Population Analysis:

Natural Population

Natural ----------

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.11034	1.99875	4.09028	0.02131	6.11034
C	2	-0.07388	1.99909	4.05684	0.01794	6.07388
C	3	-0.05057	1.99913	4.03277	0.01868	6.05057
C	4	-0.20516	1.99915	4.18672	0.01929	6.20516
C	5	-0.21549	1.99914	4.19682	0.01953	6.21549
C	6	-0.02367	1.99918	4.00587	0.01861	6.02367
H	7	0.23883	0.00000	0.75908	0.00209	0.76117
H	8	0.23452	0.00000	0.76389	0.00159	0.76548

H	9	0.23953	0.00000	0.75889	0.00159	0.76047
H	10	0.24158	0.00000	0.75680	0.00162	0.75842
C	11	0.07255	1.99899	3.90534	0.02312	5.92745
C	12	-0.15586	1.99852	4.12639	0.03096	6.15586
C	13	-0.11623	1.99879	4.09313	0.02431	6.11623
C	14	1.05353	1.99930	2.89368	0.05349	4.94647
F	15	-0.34194	1.99991	7.33239	0.00963	9.34194
F	16	-0.34195	1.99991	7.33240	0.00963	9.34195
F	17	-0.34607	1.99992	7.33641	0.00974	9.34607
H	18	0.23384	0.00000	0.76482	0.00134	0.76616
Br	19	0.16718	27.99902	6.81895	0.01485	34.83282
H	20	0.25928	0.00000	0.73851	0.00221	0.74072
H	21	0.24031	0.00000	0.75777	0.00193	0.75969

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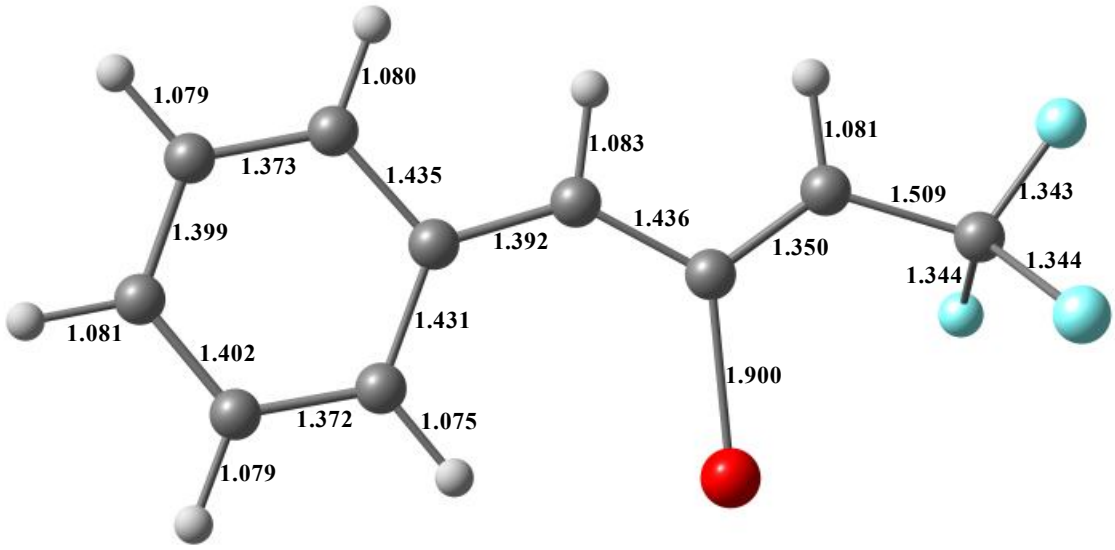
* Total *	1.00000	53.98881	73.70774	0.30345	128.00000

Bond lengths, Å

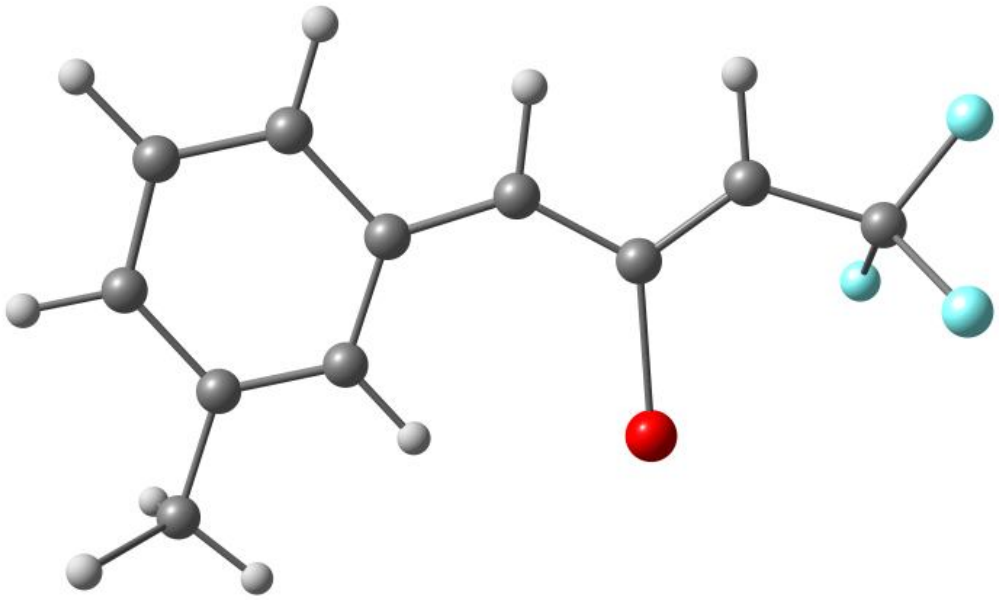


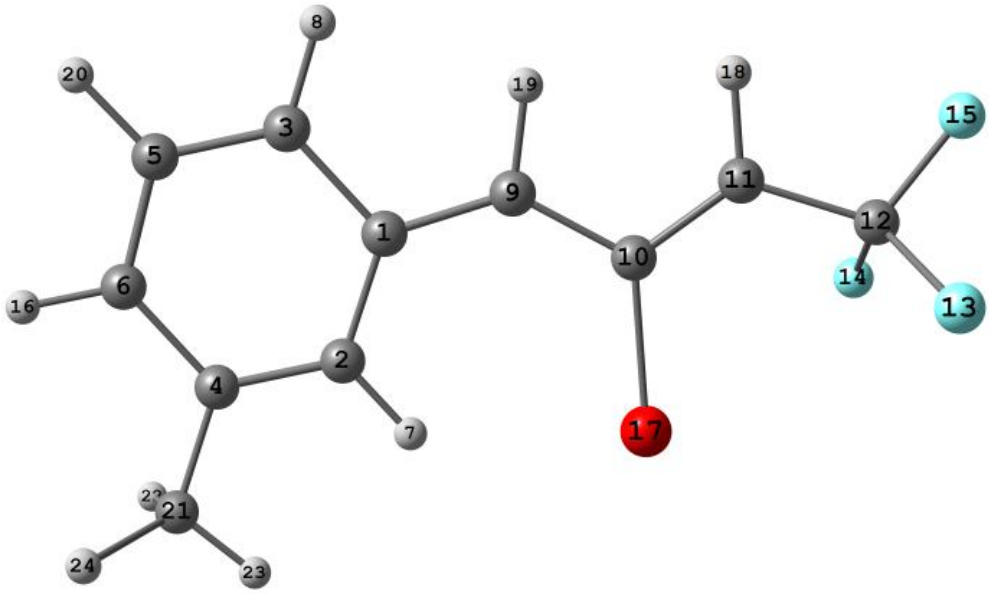
D2

E= -3298.25752232 h, G^{298}= -3298.130129 h μ= 11.93 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.756960	0.943118	-0.000733
2	C	2.357587	-0.354791	0.000991
3	C	2.610624	2.094929	-0.001751
4	C	3.725959	-0.503870	0.001687
5	C	3.974835	1.945653	-0.001230
6	C	4.522717	0.661133	0.000490
7	H	1.733371	-1.230013	0.001893
8	H	2.165217	3.078846	-0.002954
9	C	0.394913	1.226149	-0.001211
10	C	-0.805708	0.436690	-0.000860
11	C	-1.965411	1.127518	0.000363
12	C	-3.362222	0.558466	0.001469
13	F	-3.602243	-0.195388	-1.085827
14	F	-3.599974	-0.196889	1.088210
15	F	-4.255914	1.561206	0.003088
16	H	5.599524	0.552768	0.000960
17	Br	-0.811953	-1.464845	-0.002169
18	H	-1.937020	2.207420	0.000791
19	H	0.168571	2.285470	-0.001872
20	H	4.621839	2.809514	-0.002064
21	C	4.377613	-1.858794	0.003674
22	H	5.012094	-1.977487	0.882557
23	H	3.637394	-2.655042	0.004051
24	H	5.013363	-1.979468	-0.874018





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.10078	1.99875	4.08100	0.02103	6.10078
C	2	-0.09057	1.99897	4.07381	0.01779	6.09057
C	3	-0.05104	1.99912	4.03356	0.01836	6.05104
C	4	-0.02909	1.99905	4.01365	0.01640	6.02909
C	5	-0.21238	1.99914	4.19362	0.01962	6.21238

C	6	-0.01626	1.99908	3.99923	0.01794	6.01626
H	7	0.23502	0.00000	0.76254	0.00243	0.76498
H	8	0.23380	0.00000	0.76463	0.00157	0.76620
C	9	0.06622	1.99899	3.91167	0.02312	5.93378
C	10	-0.15294	1.99852	4.12360	0.03082	6.15294
C	11	-0.12340	1.99878	4.10035	0.02427	6.12340
C	12	1.05392	1.99930	2.89329	0.05350	4.94608
F	13	-0.34274	1.99991	7.33321	0.00962	9.34274
F	14	-0.34275	1.99991	7.33321	0.00962	9.34275
F	15	-0.34664	1.99992	7.33699	0.00974	9.34664
H	16	0.23056	0.00000	0.76794	0.00150	0.76944
Br	17	0.16447	27.99902	6.82163	0.01488	34.83553
H	18	0.25878	0.00000	0.73902	0.00221	0.74122
H	19	0.23963	0.00000	0.75846	0.00192	0.76037
H	20	0.24093	0.00000	0.75736	0.00171	0.75907
C	21	-0.59464	1.99928	4.58344	0.01191	6.59464
H	22	0.22946	0.00000	0.76917	0.00137	0.77054
H	23	0.22099	0.00000	0.77774	0.00127	0.77901
H	24	0.22945	0.00000	0.76918	0.00137	0.77055

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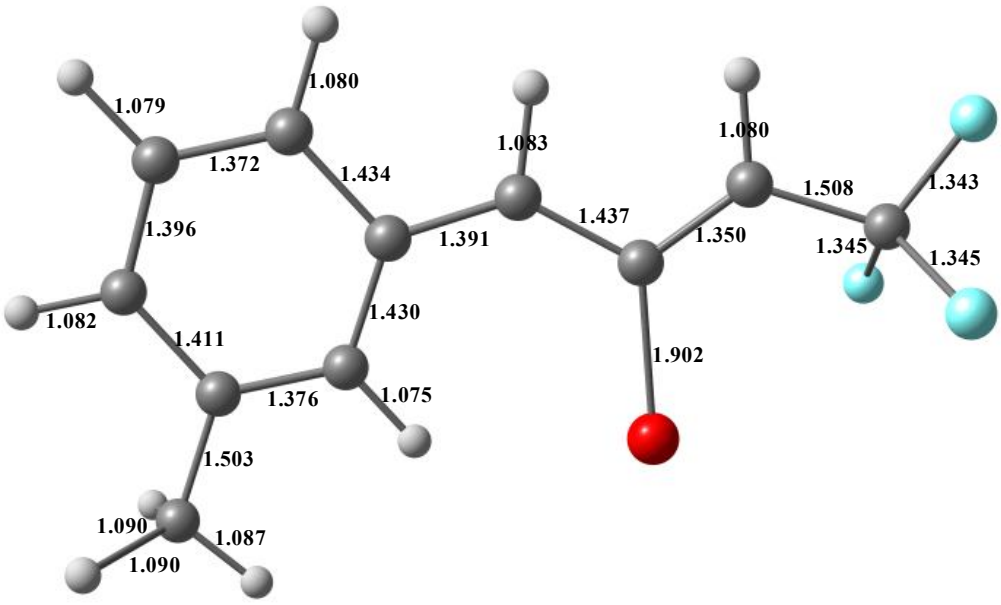
* Total *	1.00000	55.98775	79.69829	0.31395	136.00000

Bond lengths, Å

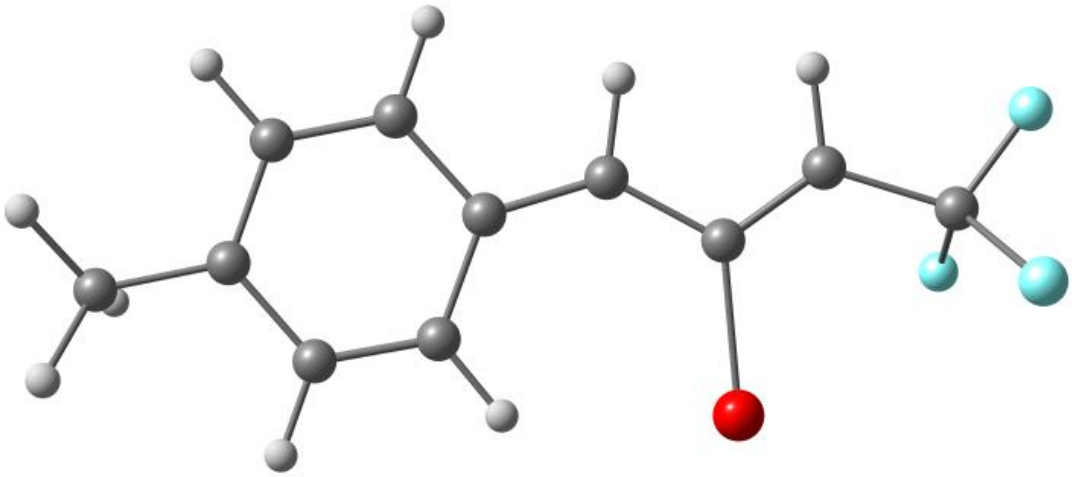


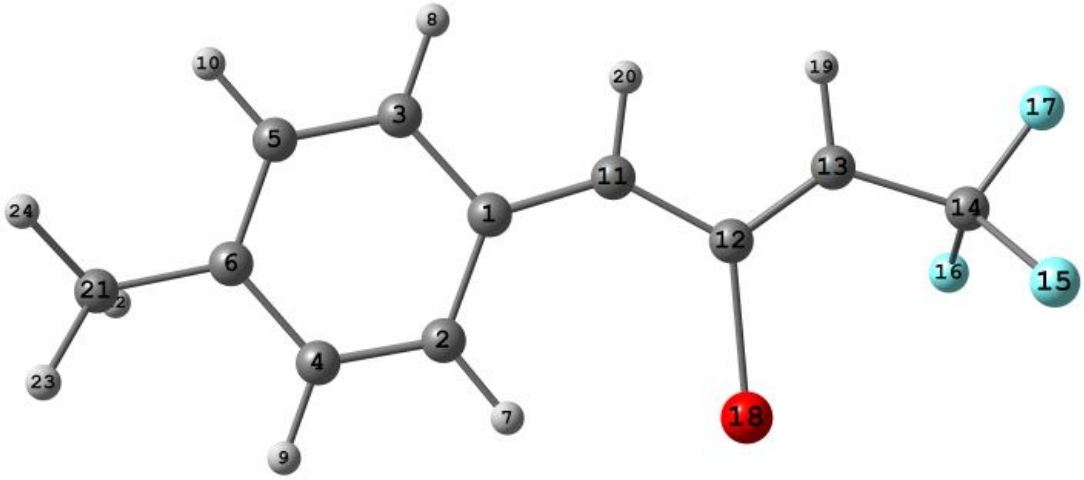
D3

E= -3298.26276615 h, G^{298}= -3298.133355 h μ= 12.92 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.708384	0.650984	-0.007875
2	C	2.204927	-0.693349	-0.014918
3	C	2.670870	1.718154	-0.003716
4	C	3.550892	-0.929041	-0.016353
5	C	4.013580	1.460997	-0.004212
6	C	4.485140	0.132946	-0.008867
7	H	1.521895	-1.523243	-0.021949
8	H	2.315416	2.738657	-0.001413
9	H	3.914765	-1.946259	-0.025878
10	H	4.721292	2.276930	-0.003929
11	C	0.380822	1.048403	-0.004742
12	C	-0.885526	0.365809	-0.001940
13	C	-1.981718	1.151528	-0.000928
14	C	-3.421404	0.706482	0.002270
15	F	-3.729798	-0.028316	-1.081489
16	F	-3.726444	-0.021437	1.091666
17	F	-4.225231	1.783730	0.000090
18	Br	-1.048932	-1.529298	0.001792
19	H	-1.860704	2.225273	-0.002294
20	H	0.244937	2.122648	-0.002526
21	C	5.945042	-0.155658	0.018852
22	H	6.244480	-0.361535	1.052244
23	H	6.185124	-1.044900	-0.561779
24	H	6.532601	0.688519	-0.333029





Summary of Natural Population Analysis:

Natural Population

Natural ----------

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.12617	1.99900	4.10783	0.01935	6.12617
C	2	-0.06997	1.99907	4.05395	0.01694	6.06997
C	3	-0.04231	1.99910	4.02569	0.01752	6.04231
C	4	-0.20630	1.99903	4.18764	0.01963	6.20630
C	5	-0.22026	1.99901	4.20147	0.01977	6.22026
C	6	0.16364	1.99909	3.82036	0.01690	5.83636
H	7	0.23917	0.00000	0.75856	0.00227	0.76083
H	8	0.23411	0.00000	0.76423	0.00166	0.76589
H	9	0.23704	0.00000	0.76111	0.00185	0.76296

H	10	0.23910	0.00000	0.75897	0.00193	0.76090
C	11	0.06273	1.99885	3.91644	0.02198	5.93727
C	12	-0.15084	1.99854	4.12140	0.03090	6.15084
C	13	-0.13942	1.99878	4.11645	0.02419	6.13942
C	14	1.05481	1.99929	2.89241	0.05349	4.94519
F	15	-0.34425	1.99991	7.33472	0.00961	9.34425
F	16	-0.34425	1.99991	7.33472	0.00961	9.34425
F	17	-0.34807	1.99992	7.33844	0.00971	9.34807
Br	18	0.15894	27.99902	6.82694	0.01510	34.84106
H	19	0.25796	0.00000	0.73987	0.00217	0.74204
H	20	0.23777	0.00000	0.76029	0.00194	0.76223
C	21	-0.61927	1.99925	4.60629	0.01373	6.61927
H	22	0.25726	0.00000	0.74120	0.00153	0.74274
H	23	0.23780	0.00000	0.76066	0.00154	0.76220
H	24	0.23078	0.00000	0.76761	0.00161	0.76922

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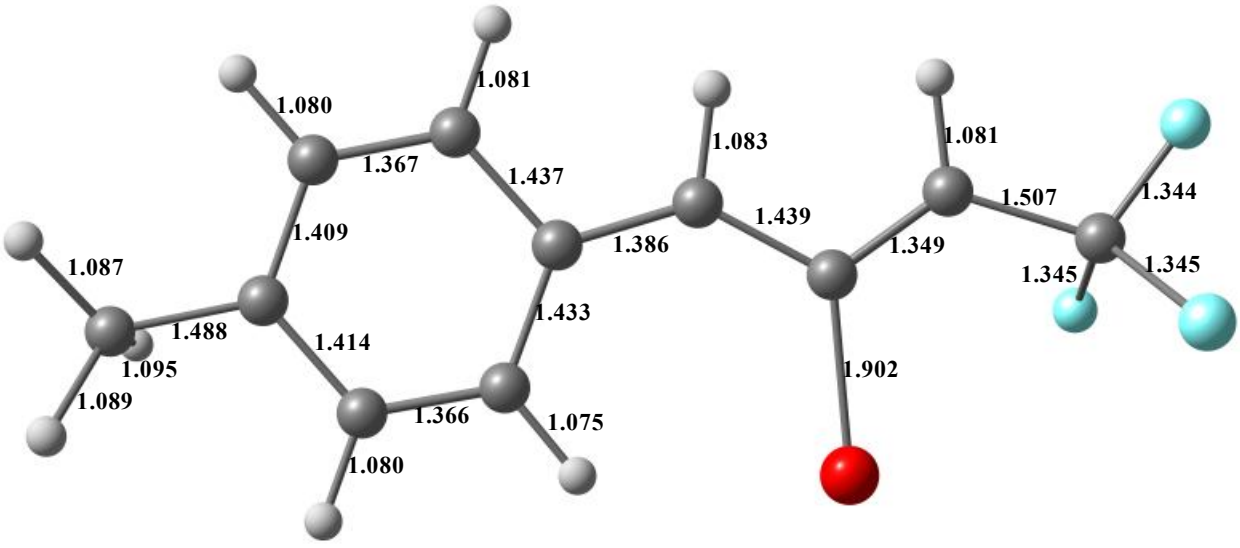
* Total *	1.00000	55.98778	79.69726	0.31496	136.00000

Bond lengths, Å

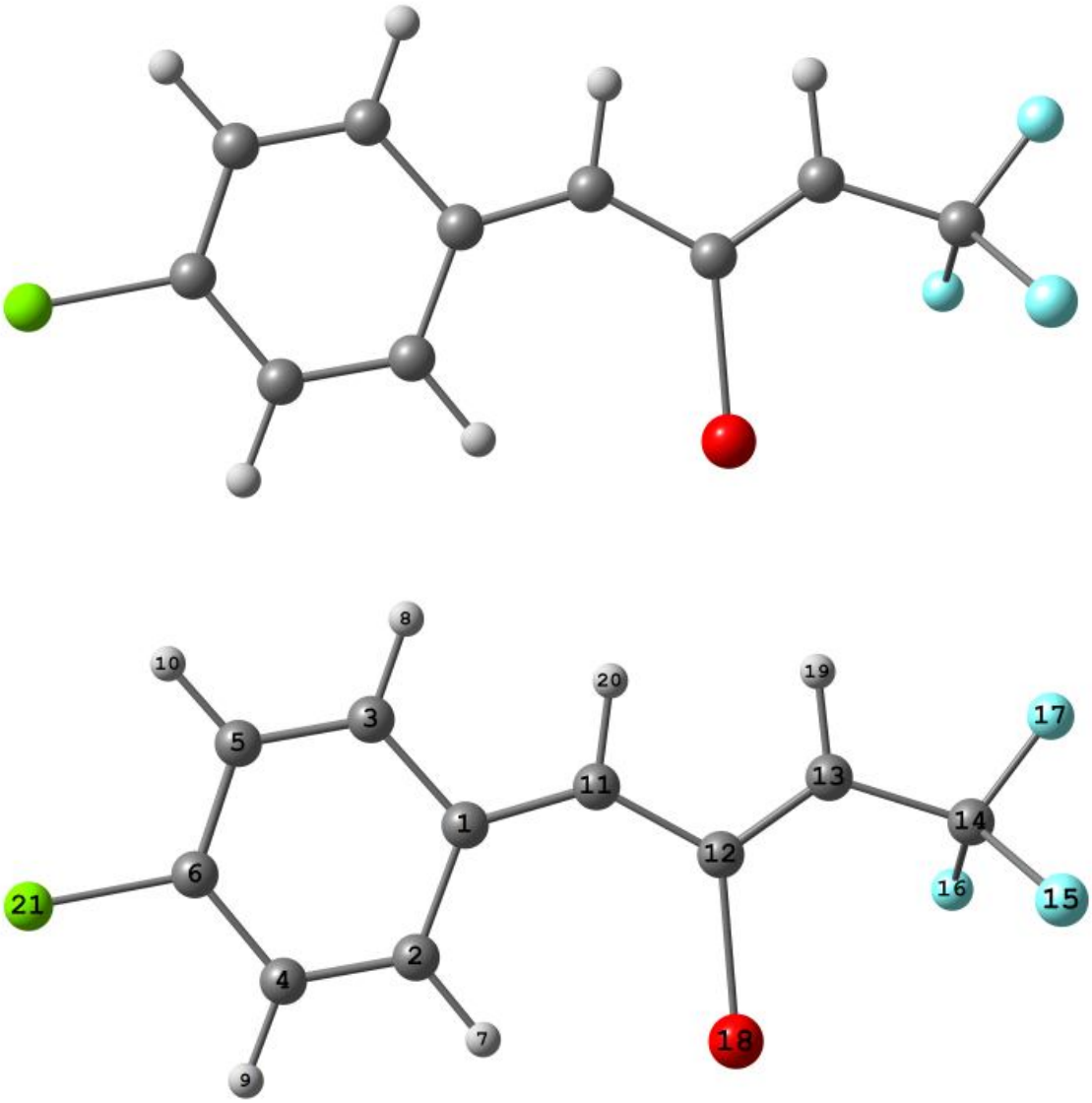


D4

E= -3718.55022003 h, G^{298}= -3718.45705 h μ= 9.06 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.363895	0.671666	-0.000239
2	C	1.864143	-0.668901	0.000360
3	C	2.315247	1.745979	-0.000782
4	C	3.211615	-0.906587	0.000409
5	C	3.662395	1.506064	-0.000768
6	C	4.106130	0.176834	-0.000162
7	H	1.186612	-1.503272	0.000822
8	H	1.955250	2.764533	-0.001228
9	H	3.593367	-1.915182	0.000887
10	H	4.373674	2.316562	-0.001187
11	C	0.029551	1.059629	-0.000297
12	C	-1.228131	0.366716	-0.000067
13	C	-2.329861	1.147276	0.000021
14	C	-3.767455	0.691879	0.000266
15	F	-4.066131	-0.041431	-1.086412
16	F	-4.065818	-0.041259	1.087149
17	F	-4.578122	1.762973	0.000297
18	Br	-1.378733	-1.528152	0.000036
19	H	-2.215852	2.221898	-0.000070
20	H	-0.113087	2.132755	-0.000590
21	Cl	5.794185	-0.141051	-0.000097



Summary of Natural Population Analysis:

Natural Population

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.10633	1.99875	4.08670	0.02088	6.10633
C	2	-0.06506	1.99909	4.04826	0.01771	6.06506
C	3	-0.04344	1.99912	4.02600	0.01833	6.04344
C	4	-0.22066	1.99896	4.19935	0.02235	6.22066
C	5	-0.23164	1.99895	4.21020	0.02249	6.23164
C	6	0.07307	1.99867	3.89875	0.02951	5.92693
H	7	0.24489	0.00000	0.75299	0.00213	0.75511
H	8	0.24072	0.00000	0.75766	0.00161	0.75928

H	9	0.25281	0.00000	0.74518	0.00201	0.74719
H	10	0.25492	0.00000	0.74302	0.00206	0.74508
C	11	0.05770	1.99899	3.92035	0.02296	5.94230
C	12	-0.15214	1.99852	4.12272	0.03089	6.15214
C	13	-0.12412	1.99878	4.10104	0.02430	6.12412
C	14	1.05380	1.99930	2.89341	0.05350	4.94620
F	15	-0.34269	1.99991	7.33315	0.00963	9.34269
F	16	-0.34269	1.99991	7.33315	0.00963	9.34269
F	17	-0.34662	1.99992	7.33698	0.00973	9.34662
Br	18	0.16517	27.99902	6.82092	0.01489	34.83483
H	19	0.25895	0.00000	0.73884	0.00220	0.74105
H	20	0.24079	0.00000	0.75729	0.00193	0.75921
Cl	21	0.13257	9.99951	6.84938	0.01854	16.86743

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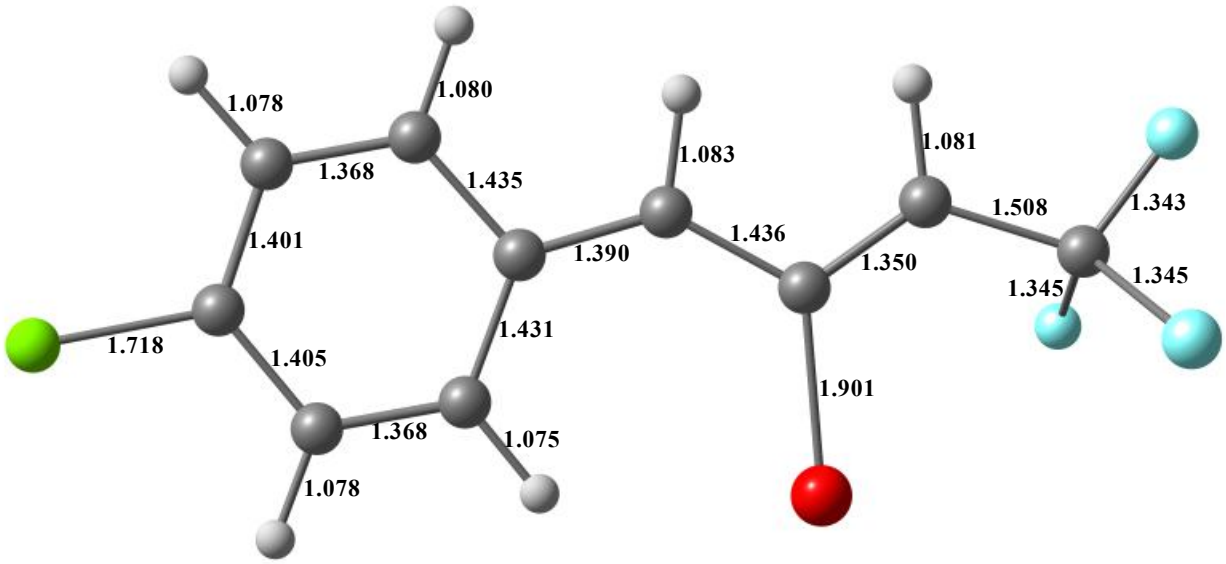
* Total *	1.00000	63.98741	79.67532	0.33727	144.00000

Bond lengths, Å

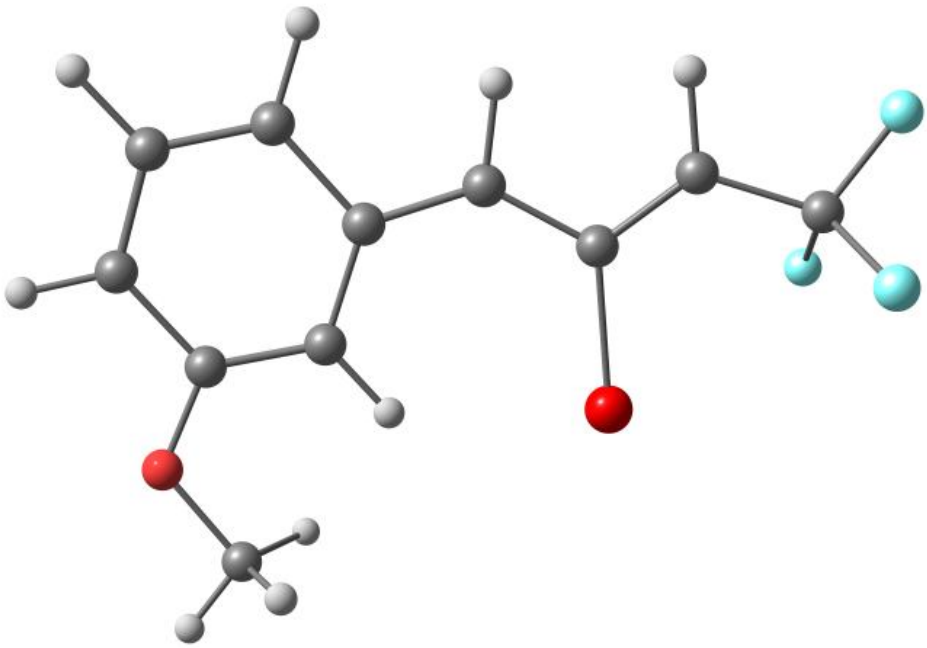


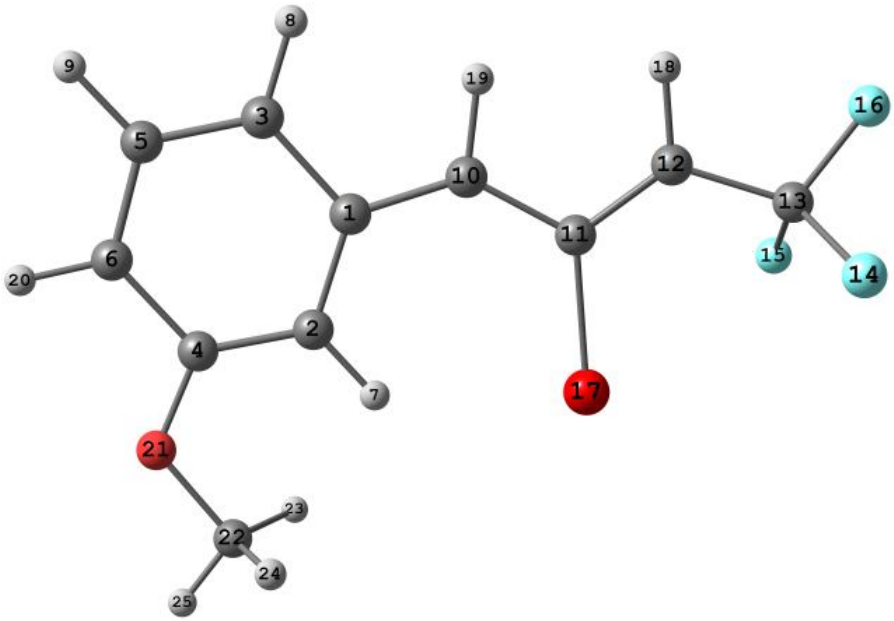
D5

E= -3373.48971504 h, G^{298}= -3373.358223 h μ= 9.86 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.479560	1.200474	-0.000049
2	C	2.169650	-0.047631	0.000080
3	C	2.231585	2.420334	-0.000221
4	C	3.548721	-0.058958	0.000014
5	C	3.607765	2.387977	-0.000321
6	C	4.261918	1.162606	-0.000207
7	H	1.613748	-0.965303	0.000252
8	H	1.705948	3.363411	-0.000292
9	H	4.179755	3.302975	-0.000478
10	C	0.098419	1.382452	-0.000023
11	C	-1.039443	0.507562	-0.000014
12	C	-2.247145	1.111295	0.000194
13	C	-3.597599	0.440798	0.000283
14	F	-3.779564	-0.329857	-1.086672
15	F	-3.779261	-0.330185	1.087059
16	F	-4.563730	1.373789	0.000558
17	Br	-0.901225	-1.389282	-0.000323
18	H	-2.296493	2.190722	0.000323
19	H	-0.205681	2.421151	-0.000011
20	H	5.342167	1.117214	-0.000272
21	O	4.318311	-1.160686	0.000145
22	C	3.677181	-2.445573	0.000388
23	H	3.066985	-2.570069	0.894565
24	H	3.066817	-2.570326	-0.893636
25	H	4.482450	-3.171152	0.000418





Summary of Natural Population Analysis:

Natural Population

Natural Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.11080	1.99902	4.09208	0.01970	6.11080
C	2	-0.19914	1.99896	4.18414	0.01604	6.19914
C	3	-0.04367	1.99911	4.02697	0.01759	6.04367
C	4	0.32349	1.99882	3.65616	0.02153	5.67651
C	5	-0.21089	1.99915	4.19214	0.01961	6.21089

C	6	-0.04667	1.99909	4.02853	0.01905	6.04667
H	7	0.24493	0.00000	0.75221	0.00286	0.75507
H	8	0.23497	0.00000	0.76346	0.00157	0.76503
H	9	0.24389	0.00000	0.75445	0.00166	0.75611
C	10	0.07663	1.99886	3.90242	0.02209	5.92337
C	11	-0.15621	1.99854	4.12662	0.03105	6.15621
C	12	-0.12420	1.99878	4.10121	0.02421	6.12420
C	13	1.05377	1.99930	2.89346	0.05347	4.94623
F	14	-0.34292	1.99991	7.33339	0.00961	9.34292
F	15	-0.34292	1.99991	7.33339	0.00961	9.34292
F	16	-0.34653	1.99992	7.33688	0.00973	9.34653
Br	17	0.16479	27.99902	6.82107	0.01513	34.83521
H	18	0.25882	0.00000	0.73902	0.00217	0.74118
H	19	0.23883	0.00000	0.75933	0.00184	0.76117
H	20	0.24217	0.00000	0.75602	0.00182	0.75783
O	21	-0.52743	1.99970	6.50391	0.02382	8.52743
C	22	-0.21237	1.99922	4.20003	0.01311	6.21237
H	23	0.18786	0.00000	0.81014	0.00200	0.81214
H	24	0.18785	0.00000	0.81015	0.00200	0.81215
H	25	0.20575	0.00000	0.79308	0.00117	0.79425

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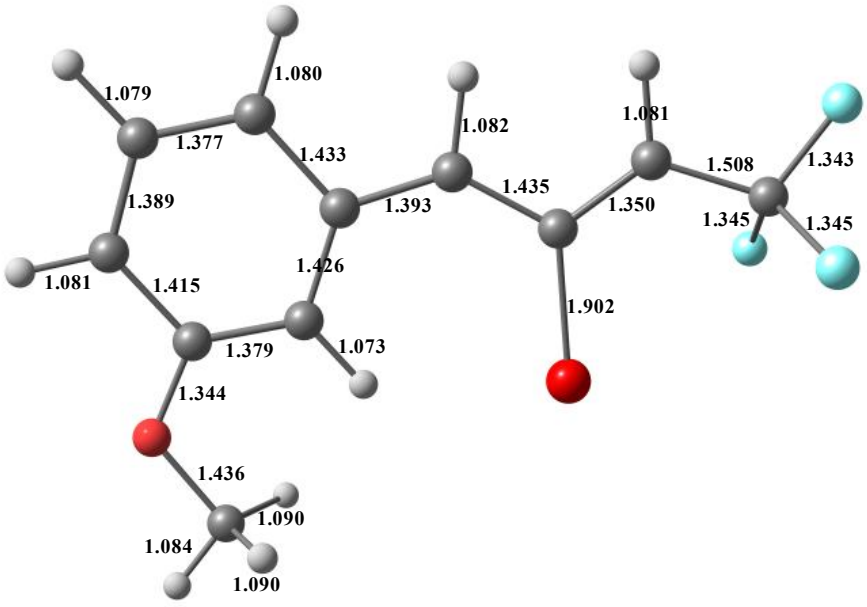
* Total *	1.00000	57.98732	85.67026	0.34242	144.00000

Bond lengths, Å

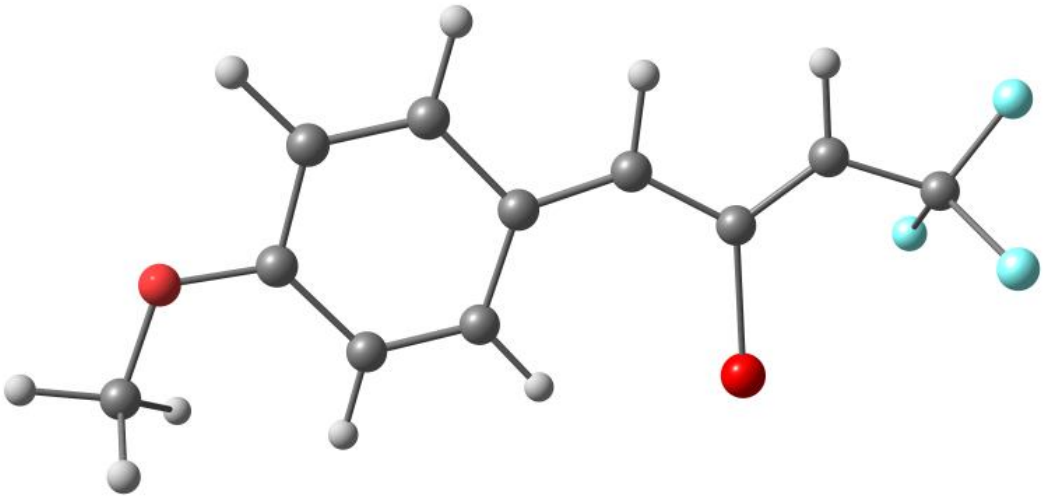


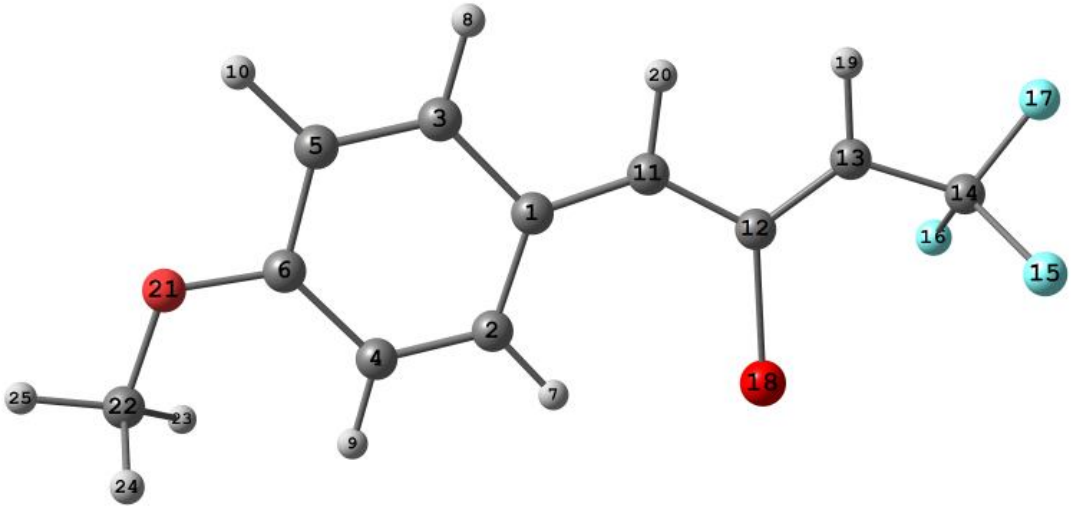
D6

E= -3373.5065995 h, G^{298}= -3373.372298 h μ= 13.46 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.327292	0.811449	-0.000098
2	C	1.890774	-0.511341	0.000043
3	C	2.249112	1.923222	-0.000185
4	C	3.237625	-0.705314	0.000097
5	C	3.591495	1.735451	-0.000139
6	C	4.113693	0.413916	0.000005
7	H	1.244054	-1.369946	0.000121
8	H	1.847559	2.926151	-0.000287
9	H	3.634372	-1.706858	0.000214
10	H	4.283763	2.563484	-0.000204
11	C	-0.011151	1.140843	-0.000125
12	C	-1.246130	0.395902	-0.000065
13	C	-2.385478	1.113318	0.000051
14	C	-3.794362	0.586071	0.000153
15	F	-4.064774	-0.163130	-1.085974
16	F	-4.064589	-0.163198	1.086281
17	F	-4.660563	1.615723	0.000259
18	Br	-1.308834	-1.508731	-0.000152
19	H	-2.327388	2.192024	0.000098
20	H	-0.202062	2.207094	-0.000193
21	O	5.419475	0.321747	0.000046
22	C	6.080183	-0.970075	0.000175
23	H	5.813068	-1.522976	0.896832
24	H	5.813072	-1.523155	-0.896372
25	H	7.137963	-0.739417	0.000155





Summary of Natural Population Analysis:

			Natural Population			
		Natural				
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.09911	1.99874	4.07944	0.02092	6.09911
C	2	-0.06723	1.99910	4.05008	0.01805	6.06723
C	3	-0.07104	1.99912	4.05354	0.01837	6.07104
C	4	-0.26691	1.99904	4.25047	0.01739	6.26691
C	5	-0.24001	1.99904	4.22059	0.02039	6.24001
C	6	0.48751	1.99895	3.49128	0.02227	5.51249
H	7	0.24088	0.00000	0.75695	0.00218	0.75912
H	8	0.23595	0.00000	0.76242	0.00163	0.76405
H	9	0.24728	0.00000	0.75077	0.00195	0.75272

H	10	0.24921	0.00000	0.74876	0.00203	0.75079
C	11	-0.00062	1.99898	3.97856	0.02309	6.00062
C	12	-0.13246	1.99852	4.10381	0.03013	6.13246
C	13	-0.17423	1.99877	4.15121	0.02426	6.17423
C	14	1.05655	1.99928	2.89064	0.05353	4.94345
F	15	-0.34773	1.99991	7.33822	0.00959	9.34773
F	16	-0.34773	1.99991	7.33823	0.00959	9.34773
F	17	-0.35092	1.99992	7.34132	0.00969	9.35092
Br	18	0.14706	27.99903	6.83891	0.01500	34.85294
H	19	0.25623	0.00000	0.74154	0.00223	0.74377
H	20	0.23750	0.00000	0.76053	0.00197	0.76250
O	21	-0.46122	1.99967	6.43670	0.02486	8.46122
C	22	-0.21502	1.99920	4.20358	0.01224	6.21502
H	23	0.20139	0.00000	0.79688	0.00172	0.79861
H	24	0.20139	0.00000	0.79688	0.00172	0.79861
H	25	0.21328	0.00000	0.78560	0.00111	0.78672

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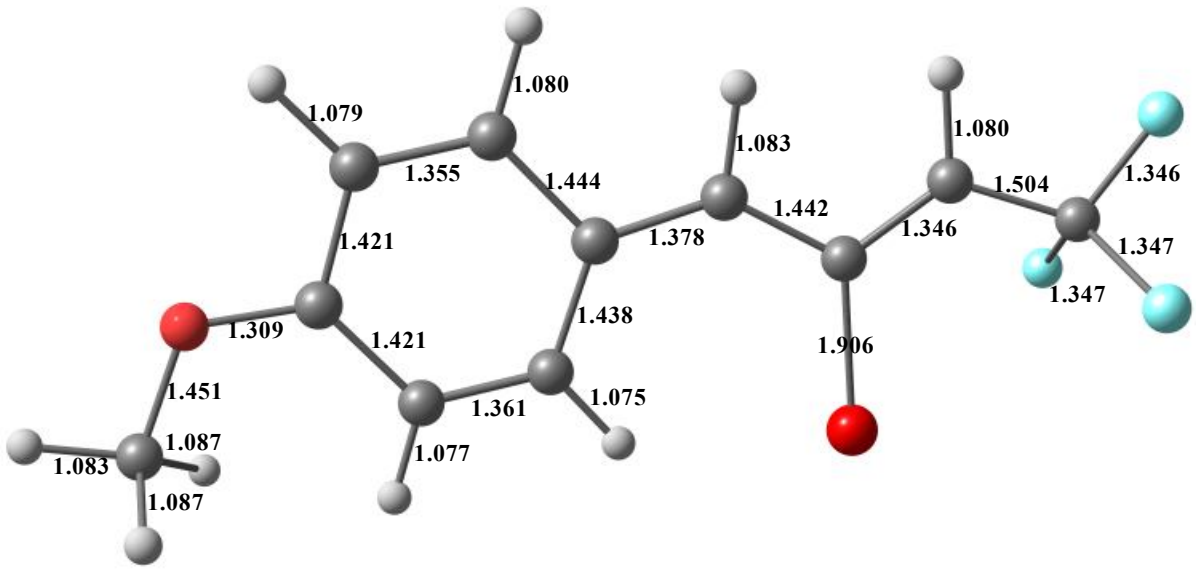
* Total *	1.00000	57.98718	85.66691	0.34591	144.00000

Bond lengths, Å

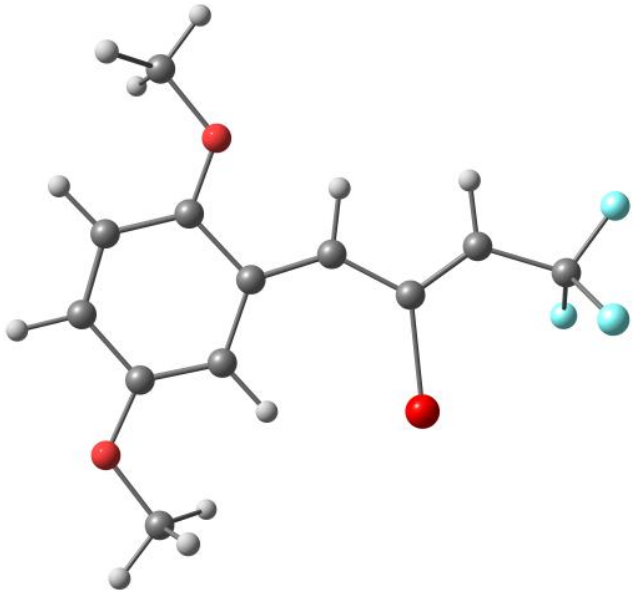


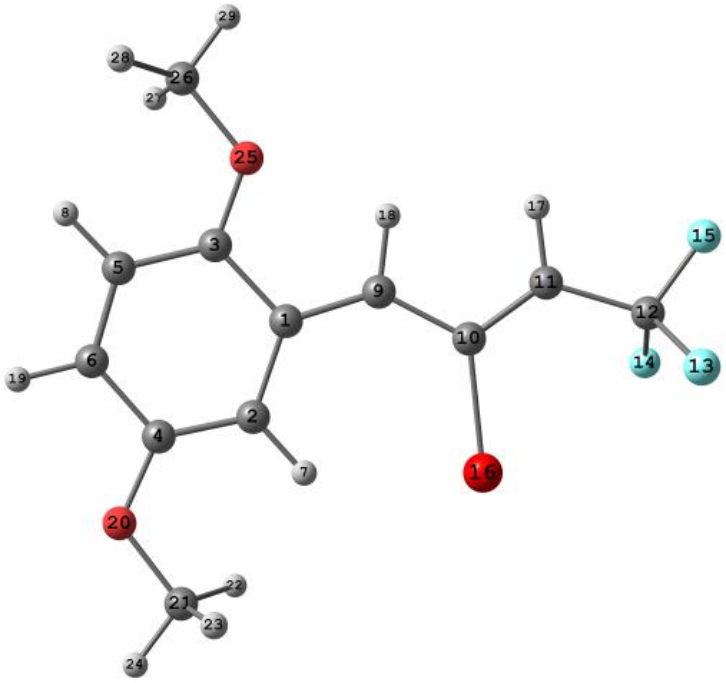
D7

E= -3488.06187968 h, G^{298}= -3487.900324 h μ= 13.01 D

Optimized geometry, A

N_{at}	Atom	x	y	z
1	C	1.386855	0.552800	-0.000042
2	C	1.851995	-0.803672	0.000036
3	C	2.388841	1.625274	-0.000126
4	C	3.188816	-1.080649	0.000027
5	C	3.754108	1.300949	-0.000135
6	C	4.134643	-0.013442	-0.000062
7	H	1.130166	-1.596782	0.000109
8	H	4.503281	2.074556	-0.000199
9	C	0.071564	0.966587	-0.000035
10	C	-1.205237	0.301815	0.000008
11	C	-2.296467	1.093302	0.000055
12	C	-3.736964	0.663944	0.000110
13	F	-4.060137	-0.065235	-1.085918
14	F	-4.060051	-0.065247	1.086155
15	F	-4.531115	1.750967	0.000146
16	Br	-1.399380	-1.595466	-0.000021
17	H	-2.165684	2.165571	0.000057
18	H	-0.053155	2.040321	-0.000069
19	H	5.184880	-0.270817	-0.000071
20	O	3.744816	-2.307107	0.000100
21	C	2.872174	-3.445624	0.000158
22	H	2.248030	-3.450225	0.893844
23	H	2.248003	-3.450295	-0.893509
24	H	3.523085	-4.312463	0.000183
25	O	1.942365	2.856757	-0.000199
26	C	2.852950	3.984562	-0.000243
27	H	3.466505	3.964135	0.896703
28	H	3.466496	3.964071	-0.897193
29	H	2.211331	4.856570	-0.000271





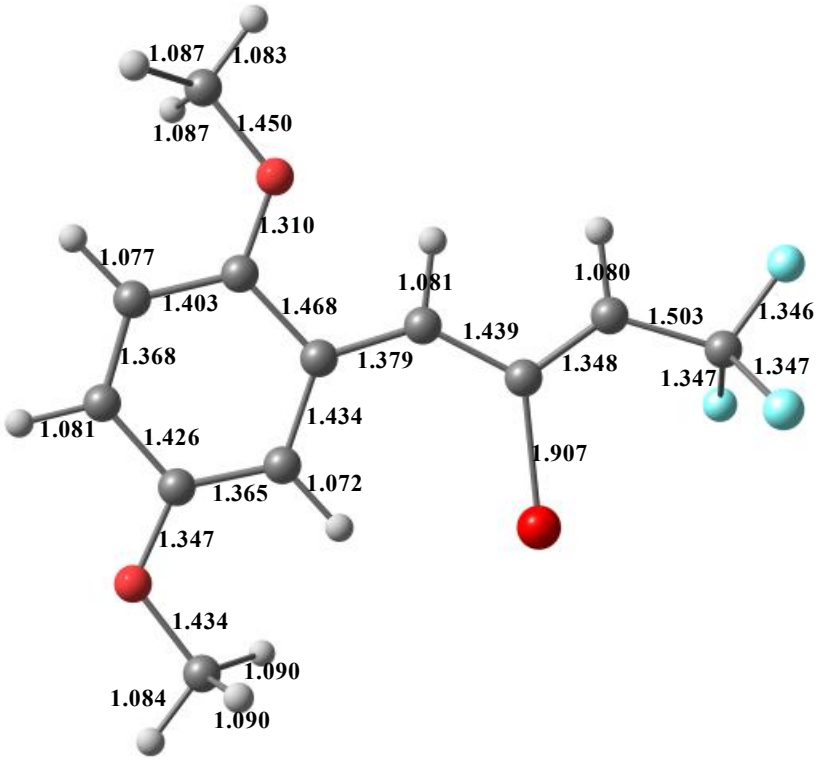
Summary of Natural Population Analysis:

Natural Population

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.11801	1.99897	4.09935	0.01970	6.11801
C	2	-0.23095	1.99891	4.21557	0.01647	6.23095
C	3	0.51107	1.99890	3.46889	0.02114	5.48893
C	4	0.31488	1.99879	3.66473	0.02160	5.68512
C	5	-0.29118	1.99904	4.27443	0.01771	6.29118

C	6	-0.03982	1.99910	4.02148	0.01925	6.03982
H	7	0.24323	0.00000	0.75395	0.00282	0.75677
H	8	0.25101	0.00000	0.74699	0.00200	0.74899
C	9	0.00080	1.99883	3.97741	0.02296	5.99920
C	10	-0.13013	1.99855	4.10158	0.03001	6.13013
C	11	-0.17926	1.99877	4.15630	0.02420	6.17926
C	12	1.05611	1.99927	2.89120	0.05342	4.94389
F	13	-0.34848	1.99991	7.33903	0.00954	9.34848
F	14	-0.34848	1.99991	7.33903	0.00954	9.34848
F	15	-0.35165	1.99992	7.34209	0.00964	9.35165
Br	16	0.14585	27.99902	6.83999	0.01514	34.85415
H	17	0.25529	0.00000	0.74250	0.00220	0.74471
H	18	0.24603	0.00000	0.75129	0.00268	0.75397
H	19	0.24410	0.00000	0.75405	0.00184	0.75590
O	20	-0.52619	1.99970	6.50263	0.02386	8.52619
C	21	-0.21178	1.99923	4.19937	0.01318	6.21178
H	22	0.18709	0.00000	0.81082	0.00209	0.81291
H	23	0.18709	0.00000	0.81082	0.00209	0.81291
H	24	0.20453	0.00000	0.79431	0.00117	0.79547
O	25	-0.47877	1.99966	6.45737	0.02174	8.47877
C	26	-0.21032	1.99920	4.19716	0.01396	6.21032
H	27	0.20183	0.00000	0.79647	0.00170	0.79817
H	28	0.20183	0.00000	0.79647	0.00170	0.79817
H	29	0.21428	0.00000	0.78470	0.00102	0.78572
* Total *		1.00000	61.98568	97.62996	0.38435	160.00000

Bond lengths, Å


1.087
1.083
1.087
1.450
1.310
1.077
1.403
1.468
1.081
1.080
1.439
1.503
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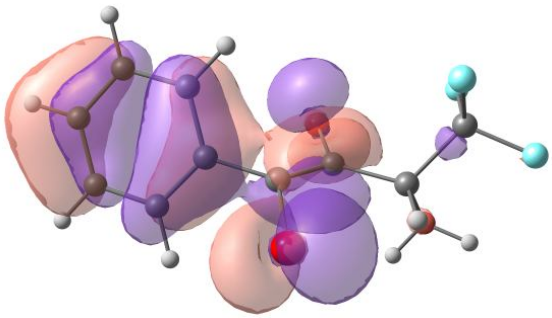
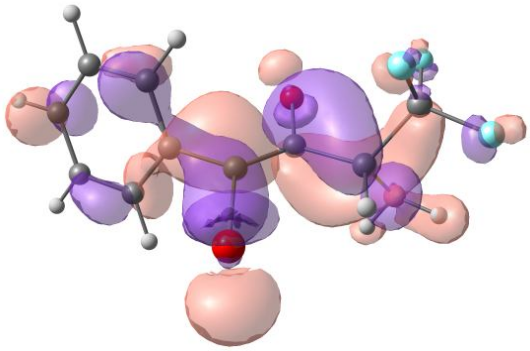
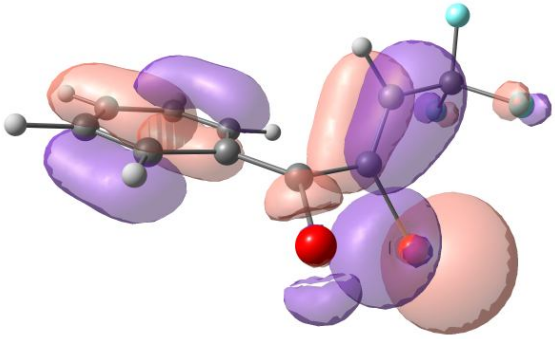
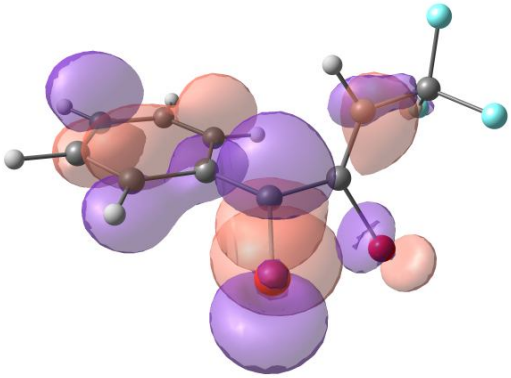
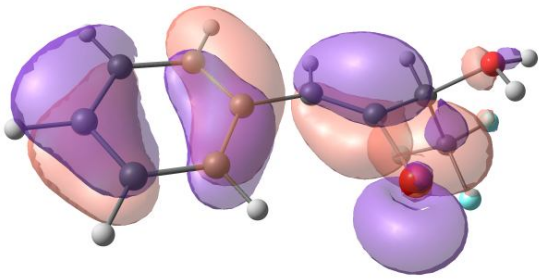
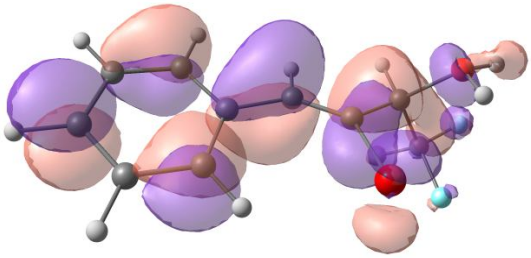
1.368
1.379
1.348
1.347
1.347
1.081
1.426
1.434
1.907
1.365
1.072
1.347
1.434
1.090
1.084
1.090

	HOMO	LUMO
A1		
B1		
C1		
D1