

Supplementary Information

Computational Insight of the Mechanism of Algar-Flynn-Oyamada (AFO) Reaction

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Table

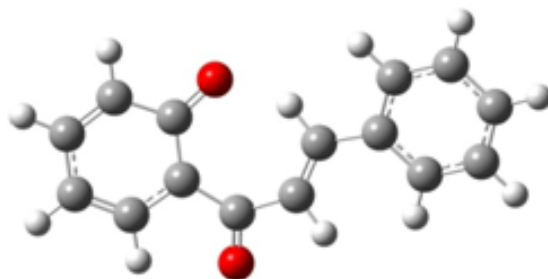
Imaginary frequency (cm⁻¹), total Energy E (a.u), Enthalpy H (a.u), Gibbs Free Energy G (a.u) and Entropy S (Cal/Mol-Kelvin) of reactant, intermediate, transition state and products at B3LYP/6-31+G(d,p)

	Imaginary Freq.	E	G	H	S
Path A					
Reactant	-	-728.543924	-728.583587	-728.528978	123.344
IM-1	-	-879.390377	-879.458090	-879.389433	144.501
TS-1	-118.90	-879.387721	-879.452091	-879.836777	137.464
IM-2	-	-879.399514	-879.462223	-879.398569	133.971
TS-2	-85.96	-879.400554	-879.461769	-879.399610	130.824
IM-3	-	-879.446092	-879.508316	-879.445148	132.949
IM-4	-	-803.732592	-803.791613	-803.731648	126.606
TS-A1	-243.98	-803.664683	-803.720854	-803.663742	120.203
IM-A1	-	-803.724203	-803.779717	-803.723249	118.827

$\cdot\text{OOH}$	-	-150.936168	-150.960904	-150.935224	54.068
$\cdot\text{OH}$	-	-75.792521	-75.811143	-75.791576	41.182
Products	-	-803.116422	-803.170738	-803.115478	116.305
Path B					
Reactant	-	-728.543924	-728.583587	-728.528978	123.344
TS-B1	-346.26	-728.505889	-728.559030	-728.504944	113.739
IM-B1	-	-728.512263	-728.566423	-728.511319	115.977
IM-B2	-	-880.072494	-880.136391	-880.071550	136.470
TS-B2	-308.96	-880.046602	-880.109188	-880.045658	133.709
IM-B3	-	-880.161512	-880.224290	-880.160568	134.114
H₂O₂	-	-151.528735	-151.553629	-151.527791	54.382
$\cdot\text{OH}$	-	-75.792521	-75.811143	-75.791576	41.182
Products	-	-803.116422	-803.170738	-803.115478	116.305
Path C					
Reactant	-	-728.543924	-728.583587	-728.528978	123.344
IM-C1	-	-880.077780	-880.148298	-880.076835	150.406
TS-C1	-318.83	-880.060495	-880.123758	-880.059551	135.134
IM-C2	-	-880.077781	-880.148322	-880.076837	150.45
H₂O₂	-	-151.528735	-151.553629	-151.527791	54.382
$\cdot\text{OH}$	-	-75.792521	-75.811143	-75.791576	41.182
Products	-	-803.116422	-803.170738	-803.115478	116.305

Path D					
Reactant	-	-728.543924	-728.583587	-728.528978	123.344
IM-1	-	-879.390377	-879.458090	-879.389433	144.501
TS-1	-118.90	-879.387721	-879.452091	-879.836777	137.464
IM-2	-	-879.399514	-879.462223	-879.398569	133.971
TS-2	-85.96	-879.400554	-879.461769	-879.399610	130.824
IM-3	-	-879.446092	-879.508316	-879.445148	132.949
IM-4	-	-803.732592	-803.791613	-803.731648	126.606
TS-D1	-423.47	-803.702853	-803.760023	-803.701909	122.320
IM-D1	-	-803.722005	-803.779327	-803.722005	120.645
\cdotOOH	-	-150.936168	-150.960904	-150.935224	54.068
\cdotOH	-	-75.792521	-75.811143	-75.791576	41.182
Aurone	-	-727.880059	-727.932892	-727.879114	113.184

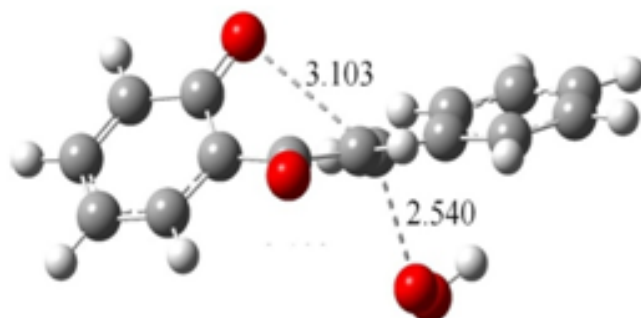
B3LYP/6-31+G(d,p) optimized geometry of the reactant, intermediate and transition state and product with selected atomic distance (\AA) and Cartesian coordinate.



Reactant

Symbol	X	Y	Z
C	-3.4580150	-1.7565610	0.0098110
C	-2.2094320	-1.0408350	0.2192000
C	-2.2814520	0.4126700	0.0533060
C	-3.5430090	0.9995690	-0.2357950
C	-4.7069020	0.2732960	-0.4149820
C	-4.6481820	-1.1358400	-0.2898410
H	-3.3975390	-2.8367130	0.1206950
H	-3.5611200	2.0811600	-0.3267000
H	-5.6409560	0.7741470	-0.6572020
H	-5.5498420	-1.7327010	-0.4308350
C	-1.1799080	1.4024800	0.1655060
O	-1.4528180	2.6195910	0.2884340
O	-1.1783880	-1.7064410	0.5520690
C	0.2891180	1.1481680	0.0429800
C	1.0179270	0.0182020	0.1485190
H	0.7889070	2.1015970	-0.1278560
H	0.4751270	-0.9093420	0.3314050
C	2.4829020	-0.0568290	0.0298020
C	3.0822200	-1.3307270	-0.0552720
C	3.3379180	1.0656070	0.0033620
C	4.4645880	-1.4798390	-0.1792150
H	2.4400730	-2.2069730	-0.0265940
C	4.7187760	0.9189550	-0.1186860
H	2.9149150	2.0617020	0.0900830
C	5.2936810	-0.3547050	-0.2137310

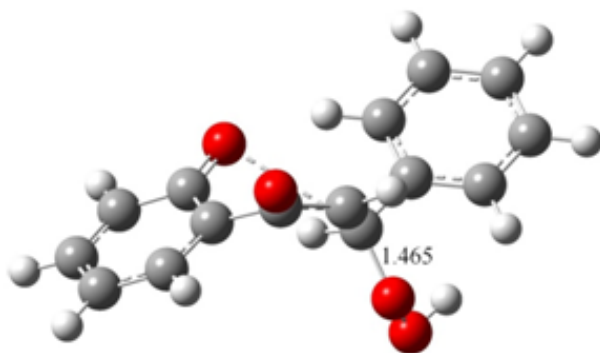
H	4.8948980	-2.4762480	-0.2466870
H	5.3527690	1.8025580	-0.1337980
H	6.3710330	-0.4660550	-0.3063160



IM-1

Symbol	X	Y	Z
C	2.4233530	1.2017440	-0.3629440
C	3.5695720	1.7377320	0.3555840
C	4.6229090	0.9597910	0.8034860
C	4.6408900	-0.4316200	0.5727890
C	3.5599000	-0.9934760	-0.1104590
C	2.4510550	-0.2520700	-0.5508530
C	1.4165880	-1.0289890	-1.3063880
C	-0.0273830	-0.8263120	-1.1519590
C	-0.6678040	-0.1333980	-0.1744750
C	-2.1124110	0.1090240	-0.1327270
C	-2.6142210	1.1852310	0.6353610
C	-3.9692650	1.5219120	0.6272610
C	-4.8808660	0.8013220	-0.1545740
C	-4.3997250	-0.2692650	-0.9261870

C	-3.0487480	-0.6033510	-0.9207450
H	3.5603140	2.8143100	0.5215450
H	5.4488220	1.4312510	1.3420140
H	5.4606560	-1.0525880	0.9293560
H	3.5495440	-2.0620840	-0.3156690
H	-0.5977330	-1.3681890	-1.9045300
H	-0.0827560	0.4109030	0.5555610
H	-1.9175800	1.7515890	1.2453830
H	-4.3150160	2.3564680	1.2360020
H	-5.9378470	1.0609890	-0.1605770
H	-5.0914380	-0.8528990	-1.5328340
H	-2.7069230	-1.4495320	-1.5077890
O	1.7936210	-1.9296280	-2.0952420
O	1.5194050	1.9759350	-0.8045370
O	-1.5109840	-1.5461300	1.7613410
O	-2.1475490	-0.8688540	2.9118890
H	-2.9670490	-0.5471800	2.5032030

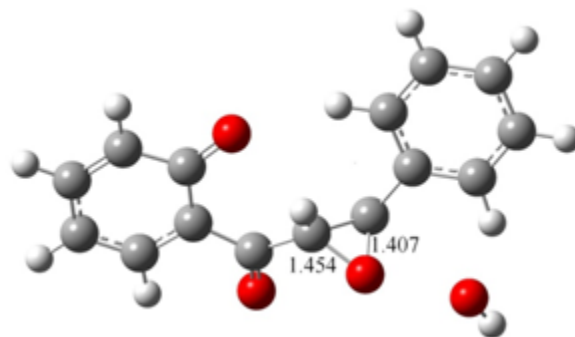


IM-2

Symbol	X	Y	Z
C	4.5534680	-0.2404960	0.4161340

C	3.4825750	-0.8032600	-0.2947170
C	2.2484430	-0.1679150	-0.4757830
C	2.0528640	1.1812310	0.0501210
C	3.1845690	1.7302100	0.7674030
C	4.3823210	1.0492080	0.9481710
H	5.4861650	-0.7880170	0.5475150
H	3.5980690	-1.7861100	-0.7487680
C	1.2454410	-0.9218060	-1.3409330
H	3.0505610	2.7353480	1.1674580
H	5.1938260	1.5233530	1.5068560
O	1.6908030	-1.4129960	-2.4290900
O	0.9853220	1.8753090	-0.0978210
C	-0.7335500	-0.6823090	0.3043310
H	-0.0905880	-0.0131410	0.8782300
C	-0.1044700	-1.1010160	-0.9566240
H	-0.7419670	-1.6032790	-1.6827430
O	-0.8879070	-1.9444170	1.0330820
O	-1.5106840	-1.7096450	2.4721040
H	-2.3914580	-1.3912040	2.2123830
C	-2.0815190	-0.0196340	0.0767650
C	-2.1472970	1.3798170	-0.0804000
C	-3.2709000	-0.7624170	-0.0343410
C	-3.3664130	2.0061990	-0.3370790
H	-1.2091440	1.9317430	-0.0302180
C	-4.4934510	-0.1302750	-0.3018080
H	-3.2194680	-1.8435070	0.0722410
C	-4.5515400	1.2581210	-0.4492470

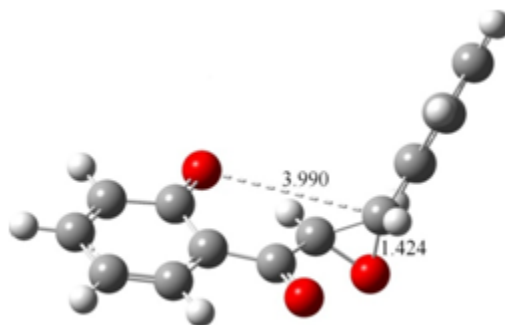
H	-3.3973680	3.0882880	-0.4582320
H	-5.4014870	-0.7263510	-0.3921160
H	-5.5006690	1.7529220	-0.6507700



IM-3

Symbol	X	Y	Z
C	2.4497820	-1.1286570	0.1521050
C	3.7407900	-1.7999710	0.1939330
C	4.9416710	-1.1407910	0.0196680
C	4.9740720	0.2556810	-0.2016770
C	3.7646070	0.9431960	-0.2281340
C	2.5141310	0.3207160	-0.0383660
C	1.3264410	1.2252980	-0.0656970
C	0.0147880	0.7273970	0.4849790
C	-1.2566050	0.8945730	-0.2695140
C	-2.3346150	-0.1538930	-0.1771060
C	-2.0128080	-1.5185680	-0.2376400
C	-3.0316160	-2.4815780	-0.2053060
C	-4.3696110	-2.0847490	-0.1034640
C	-4.6819190	-0.7194440	-0.0285840
C	-3.6771480	0.2534730	-0.0650890
H	3.7090170	-2.8766250	0.3531640

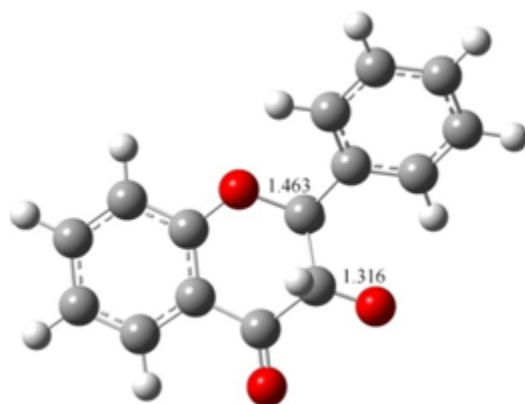
H	5.8759380	-1.7058380	0.0517160
H	5.9182240	0.7799440	-0.3365220
H	3.7470110	2.0180770	-0.3935800
H	0.0877270	-0.1324560	1.1443730
H	-1.2321360	1.4551270	-1.2053560
H	-0.9680830	-1.8203830	-0.2910020
H	-2.7750290	-3.5391690	-0.2496870
H	-5.1620630	-2.8338100	-0.0754850
H	-5.7238040	-0.4098610	0.0633680
H	-3.8428700	1.3519230	-0.0029220
O	1.4219700	2.3818100	-0.4963560
O	1.3773930	-1.8016810	0.2547410
O	-0.9920550	1.7131110	0.8450460
O	-3.0976890	2.9961920	0.1123500
H	-3.4826520	3.8415170	-0.1649480



IM-4

Symbol	X	Y	Z
C	4.7861290	0.1487770	0.5037860
C	3.6125500	0.8679110	0.3782230

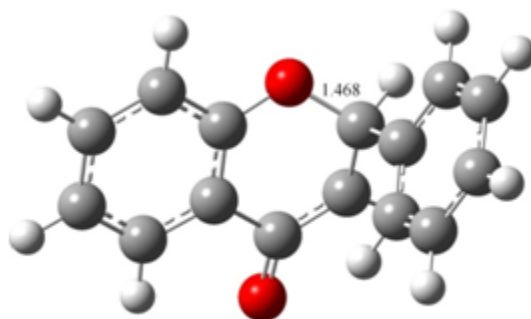
C	2.3725720	0.2688000	0.0360190
C	2.2979900	-1.1827780	-0.1613090
C	3.5684000	-1.8842970	-0.0441560
C	4.7465840	-1.2526050	0.2796730
H	5.7196190	0.6441330	0.7585010
H	3.6061540	1.9437310	0.5326910
C	1.2354130	1.1813930	-0.1004100
H	3.5312260	-2.9588070	-0.2080550
H	5.6632410	-1.8368630	0.3671450
C	-1.3437560	1.1854660	-0.0112490
C	-0.0930710	0.6440090	-0.6096150
H	-0.0984040	-0.3691740	-0.9990150
O	1.2969120	2.3926250	0.1707570
O	1.2361710	-1.8341380	-0.3991000
C	-2.5975040	0.3863850	0.0993960
C	-3.1511530	-0.2625990	-1.0142340
C	-3.2482300	0.2765260	1.3370630
C	-4.3203890	-1.0138590	-0.8874660
H	-2.6536640	-0.1653610	-1.9739820
C	-4.4168090	-0.4780490	1.4659740
H	-2.8301020	0.7820250	2.2045060
C	-4.9586040	-1.1271720	0.3526950
H	-4.7349500	-1.5145690	-1.7589230
H	-4.9041440	-0.5575060	2.4345990
H	-5.8679370	-1.7147340	0.4498220
H	-1.2022210	1.9519030	0.7529100
O	-0.9292770	1.5974840	-1.3099730



IM-A1

Symbol	X	Y	Z
C	-4.4058280	-0.7541100	0.0029930
C	-3.6436580	0.4086960	-0.0808530
C	-2.2410430	0.3702360	-0.0531130
C	-1.6026180	-0.8765970	0.0866630
C	-2.3644390	-2.0557290	0.1764420
C	-3.7544420	-1.9912370	0.1276520
H	-5.4911300	-0.7060450	-0.0306170
H	-4.1076220	1.3858310	-0.1830270
C	-1.4366560	1.6371540	-0.1745250
H	-1.8439280	-3.0021760	0.2885220
H	-4.3344660	-2.9088520	0.1963410
C	0.5307110	0.1831630	0.4266700
C	0.0903090	1.4729980	-0.3965240
C	1.9791440	-0.1835050	0.2149010
C	2.9781180	0.7409760	0.5745520
C	2.3685530	-1.4094880	-0.3445240
C	4.3263920	0.4362960	0.3766710

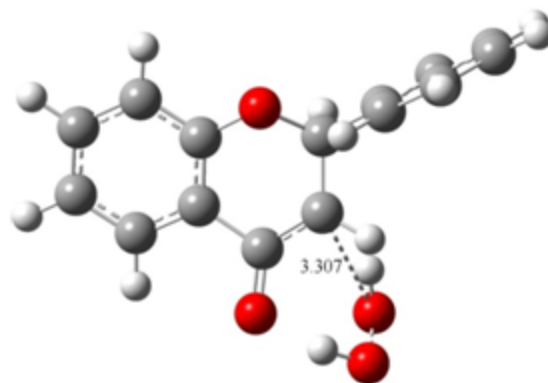
H	2.6616060	1.7065620	0.9531350
C	3.7218430	-1.7136350	-0.5339360
H	1.6079620	-2.1267900	-0.6307920
C	4.7086020	-0.7931970	-0.1728780
H	5.0838930	1.1684360	0.6477720
H	4.0007420	-2.6723360	-0.9663530
H	5.7606300	-1.0282590	-0.3196470
O	-0.2596020	-1.0111920	0.1277740
O	-2.0049870	2.7216250	-0.1532210
O	0.8489160	2.5183170	-0.1430340
H	0.0940940	1.1035190	-1.4780200
H	0.3636680	0.4179770	1.4893940



IM-B1

Symbol	X	Y	Z
C	3.4637550	-1.1821690	0.9941490
C	2.9322380	0.1076970	0.8956030
C	1.8367380	0.3886550	0.0712090
C	1.2724370	-0.6709620	-0.6671060
C	1.8027700	-1.9650090	-0.5884370

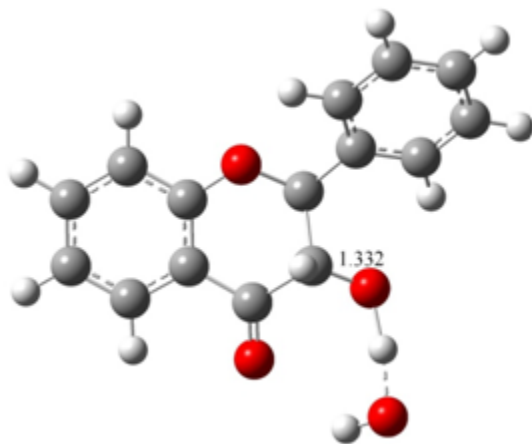
C	2.8973920	-2.2195110	0.2438600
H	4.3154890	-1.3768580	1.6423620
H	3.3570470	0.9496720	1.4353600
C	1.3212090	1.8010300	-0.0815940
H	3.3003450	-3.2283430	0.3067950
C	-0.6100910	0.7067340	-1.3043210
C	0.1633980	1.8991600	-0.8443800
H	-0.2712140	2.8765030	-1.0400620
C	-1.7817770	0.2503300	-0.4101320
C	-1.7887280	0.4809550	0.9716550
C	-2.8737640	-0.4221750	-0.9785510
C	-2.8471310	0.0308290	1.7658830
H	-0.9608510	1.0337390	1.4060100
C	-3.9427990	-0.8619720	-0.1930790
H	-2.8804650	-0.6048270	-2.0519240
C	-3.9307040	-0.6397280	1.1880030
H	-2.8303590	0.2117170	2.8383670
H	-4.7831870	-1.3754670	-0.6557810
H	-4.7598370	-0.9781960	1.8052190
O	0.2260580	-0.4797130	-1.5245300
H	1.3448930	-2.7538360	-1.1791700
H	-1.0405470	0.8858750	-2.2993560
O	1.9888210	2.7468180	0.4514810



IM-B2

Symbol	X	Y	Z
C	4.1830080	-1.4900140	-0.0753230
C	3.4786890	-0.3022000	0.1388590
C	2.0795890	-0.2718490	0.1148330
C	1.3166100	0.9741120	0.4582940
C	-0.0474910	0.9103710	0.2192330
C	-0.6398980	-0.2678380	-0.5021850
C	-2.1166780	-0.4521310	-0.2157820
C	-3.0737820	-0.1450280	-1.1888210
C	-4.4408260	-0.2708930	-0.9171430
C	-4.8648630	-0.7234010	0.3342490
C	-3.9133340	-1.0411200	1.3109970
C	-2.5515150	-0.8992900	1.0399640
H	1.5142930	-3.5852820	-0.4973970
H	4.0146790	-3.6117020	-0.4623930
H	5.2700890	-1.4928690	-0.0567880
H	3.9859690	0.6332340	0.3551110
H	-0.7116150	1.6930540	0.5734970
H	-0.5200490	-0.2030400	-1.6015500

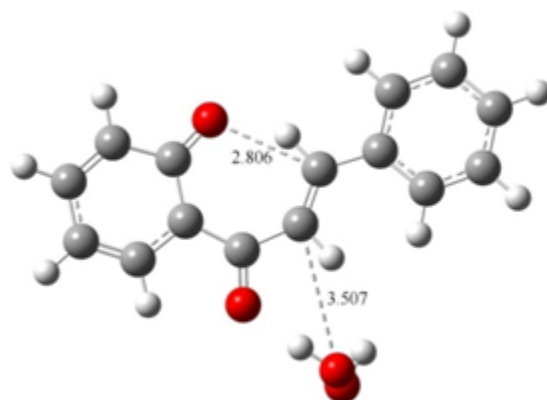
H	-2.7450890	0.1996790	-2.1665870
H	-5.1701310	-0.0193560	-1.6832690
H	-5.9256370	-0.8273930	0.5487530
H	-4.2351560	-1.3940610	2.2878360
H	-1.8092810	-1.1349300	1.7959380
O	0.0212380	-1.5267230	-0.1433390
O	1.9738860	1.9538270	0.9717890
O	0.5899850	3.9043410	-1.0347780
H	0.2002010	3.0084660	-1.0041130
O	0.7514240	4.1923900	0.3901160
H	1.2980940	3.3896620	0.6899800



IM-B3

Symbol	X	Y	Z
C	-1.6082380	-1.2311630	0.0329200
C	-2.3692930	-2.4131080	-0.0063920
C	-3.7588620	-2.3423730	-0.0336680
C	-4.4115230	-1.0992080	-0.0111430
C	-3.6512660	0.0659090	0.0280770

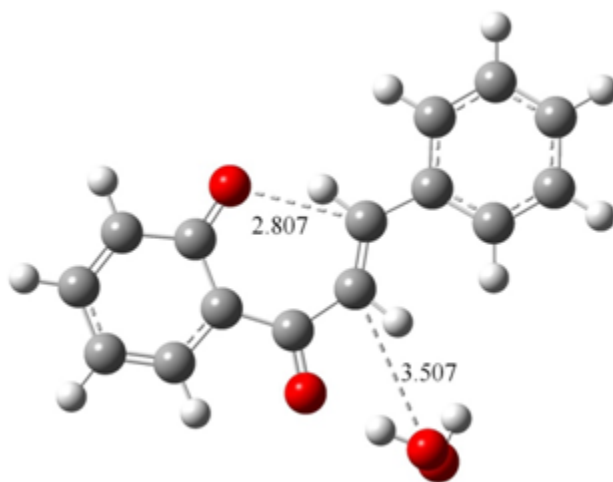
C	-2.2479910	0.0224740	0.0402090
C	-1.4406740	1.2858000	0.0418560
C	0.0851510	1.1375200	-0.1803830
C	0.5270510	-0.2209430	0.4862250
C	1.9784260	-0.5630320	0.2362690
C	2.9788030	0.2891300	0.7375520
C	4.3268780	0.0040070	0.5130370
C	4.7048140	-1.1350200	-0.2071120
C	3.7160040	-1.9841430	-0.7083630
C	2.3630900	-1.6990010	-0.4900610
H	-1.8488230	-3.3659500	-0.0086260
H	-4.3392850	-3.2615350	-0.0645280
H	-5.4967660	-1.0490480	-0.0288030
H	-4.1162060	1.0475480	0.0384610
H	0.1255480	0.9292190	-1.2941460
H	0.3591900	-0.1120570	1.5687640
H	2.6696850	1.1912920	1.2531030
H	5.0862840	0.6813580	0.8964750
H	5.7563570	-1.3547070	-0.3774320
H	3.9926910	-2.8713410	-1.2737450
H	1.6006900	-2.3613930	-0.8836310
O	-0.2642040	-1.3673630	0.0469700
O	-1.9978170	2.3712350	0.1602950
O	0.8394100	2.1537350	0.2353370
H	0.4771380	3.6828150	-0.3589840
O	0.0993280	4.5572780	-0.6768630
H	-0.8344670	4.4236290	-0.4669520



IM-C1

Symbol	X	Y	Z
C	-2.2853830	-1.5965320	0.2428950
C	-3.5667670	-2.2857630	0.1855120
C	-4.7522540	-1.6565580	-0.1006780
C	-4.7758070	-0.2634500	-0.3680720
C	-3.5870050	0.4356280	-0.3424910
C	-2.3209360	-0.1635860	-0.0719910
C	-1.1910020	0.7761300	-0.1448260
C	0.2649540	0.4753950	-0.2149740
C	0.9702440	-0.6421240	0.0622210
C	2.4341530	-0.7601330	-0.0314390
C	3.0171400	-2.0134970	0.2465830
C	4.3980490	-2.2062060	0.1792060
C	5.2388780	-1.1454000	-0.1687200
C	4.6788250	0.1078010	-0.4476230
C	3.2999400	0.2986580	-0.3800980
H	-3.5287880	-3.3500310	0.4039240
H	-5.6793770	-2.2294610	-0.1213200

H	-5.7094220	0.2428580	-0.5988300
H	-3.5829940	1.5002360	-0.5495590
H	0.7991910	1.3732390	-0.5206070
H	0.4122970	-1.5221260	0.3776400
H	2.3645720	-2.8394650	0.5166050
H	4.8170530	-3.1852460	0.3984760
H	6.3149020	-1.2897480	-0.2215250
H	5.3221330	0.9415080	-0.7184210
H	2.8911730	1.2803180	-0.5986740
O	-1.4428080	2.0162110	-0.2346040
O	-1.2612140	-2.2645250	0.5792220
O	0.3472350	3.9806800	-0.3198860
H	-0.3666920	3.2737420	-0.2759760
O	0.3578780	4.4865340	1.0464700
H	0.9990490	3.8908090	1.4656250

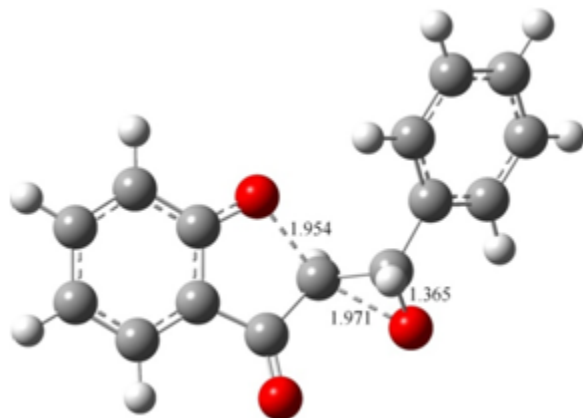


IM-C2

Symbol	X	Y	Z
C	-2.2859980	-1.5942020	0.2470840

C	-3.5668640	-2.2841650	0.1878160
C	-4.7517700	-1.6562070	-0.1036160
C	-4.7751710	-0.2638690	-0.3749350
C	-3.5867200	0.4358050	-0.3478400
C	-2.3212680	-0.1622760	-0.0722330
C	-1.1913370	0.7774320	-0.1446740
C	0.2644400	0.4760930	-0.2157590
C	0.9695200	-0.6409640	0.0637960
C	2.4332190	-0.7601010	-0.0316130
C	3.0157310	-2.0135260	0.2471330
C	4.3964090	-2.2072710	0.1780370
C	5.2374950	-1.1474480	-0.1722590
C	4.6779290	0.1058380	-0.4517490
C	3.2992670	0.2977150	-0.3825790
H	-3.5291530	-3.3477850	0.4094160
H	-5.6785890	-2.2295590	-0.1254030
H	-5.7083150	0.2413460	-0.6099460
H	-3.5825150	1.4998440	-0.5578750
H	0.7986500	1.3728740	-0.5245810
H	0.4115040	-1.5196880	0.3826970
H	2.3629750	-2.8387290	0.5190380
H	4.8150400	-3.1863500	0.3978470
H	6.3133460	-1.2925960	-0.2263590
H	5.3214450	0.9388250	-0.7242600
H	2.8908930	1.2794610	-0.6015200
O	-1.4429840	2.0174810	-0.2347110
O	-1.2624780	-2.2604000	0.5889620

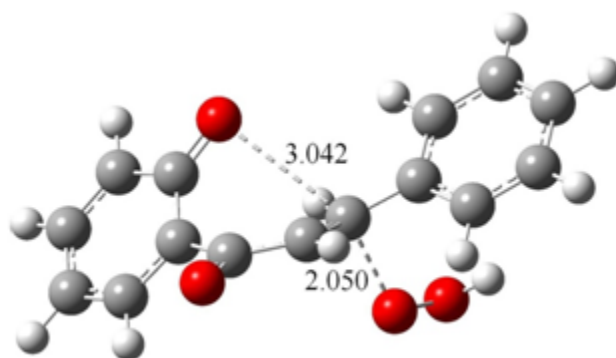
O	0.3486740	3.9808420	-0.3170670
H	-0.3658470	3.2744800	-0.2741430
O	0.3638180	4.4806700	1.0514520
H	1.0050400	3.8820200	1.4663530



IM-D1

Symbol	X	Y	Z
C	-1.7666040	-0.2948330	-0.7543110
C	-1.5959090	-0.4153880	0.6306600
C	-2.3636990	0.3505340	1.5095610
C	-3.2972130	1.2445140	0.9802620
C	-3.4524630	1.3606210	-0.4150000
C	-2.6906800	0.5987210	-1.3049000
C	-0.0868740	-1.8336860	-0.5266720
C	-0.5798200	-1.4675990	0.8488750
H	-2.2226660	0.2419590	2.5815940
H	-3.9045820	1.8572300	1.6410220
H	-4.1838080	2.0609550	-0.8120220
H	-2.8075760	0.6872030	-2.3806390

O	-0.2154320	-1.9300880	1.9284790
O	-0.9705950	-1.1232390	-1.4632230
C	1.5243000	-1.4891010	-0.8499020
H	-0.1422050	-2.8974140	-0.7556280
C	1.8213410	-0.0323900	-0.4247720
C	1.4516770	1.0732150	-1.2033680
C	2.5373690	0.1929760	0.7586910
C	1.7684400	2.3761820	-0.8023770
H	0.9161150	0.9083280	-2.1362490
C	2.8529980	1.4911080	1.1669560
H	2.8415740	-0.6838400	1.3232950
C	2.4692550	2.5910630	0.3889180
H	1.4723910	3.2221050	-1.4203260
H	3.4054890	1.6493850	2.0915760
H	2.7196560	3.6021400	0.7036290
H	1.4537180	-1.4746430	-1.9723560
O	2.2984250	-2.4028010	-0.3252100

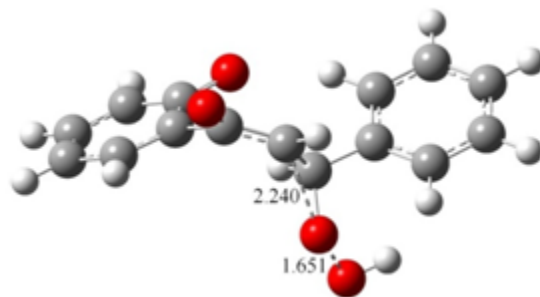


TS-1

Symbol	X	Y	Z
C	2.2916580	1.1310380	-0.4300550

C	3.4432630	1.8401890	0.1008300
C	4.5642080	1.2086430	0.6174260
C	4.6458200	-0.1967080	0.6404540
C	3.5630240	-0.9216610	0.1285190
C	2.3950180	-0.3301250	-0.3739370
C	1.3803970	-1.2979980	-0.9404940
C	-0.0430930	-1.1667280	-0.7423290
C	-0.6988400	-0.2723470	0.0877230
C	-2.1204980	0.0596520	-0.1397300
C	-2.5367500	1.4046600	-0.1275400
C	-3.8682720	1.7567730	-0.3704450
C	-4.8283380	0.7713600	-0.6246410
C	-4.4318380	-0.5745170	-0.6252680
C	-3.1028530	-0.9235950	-0.3822170
H	3.3808590	2.9278080	0.0713600
H	5.3890820	1.8098140	1.0092920
H	5.5174180	-0.7067050	1.0481550
H	3.6074200	-2.0089040	0.1079470
H	-0.6252610	-1.8863040	-1.3173860
H	-0.1164570	0.5205220	0.5372900
H	-1.7885780	2.1713520	0.0528380
H	-4.1563140	2.8070980	-0.3605320
H	-5.8664240	1.0425010	-0.8098100
H	-5.1685480	-1.3565500	-0.8059250
H	-2.8054950	-1.9667830	-0.3488750
O	1.8185280	-2.2761030	-1.6089450
O	1.3091620	1.7798480	-0.9178500

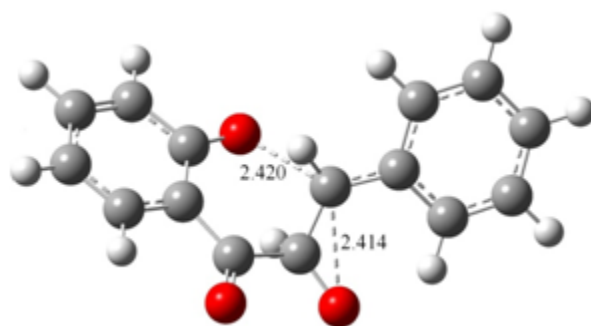
O	-1.0692250	-1.2360240	1.8589000
O	-1.8748010	-0.4868410	2.8506510
H	-2.7544540	-0.5327040	2.4438120



TS-2

Symbol	X	Y	Z
C	2.0565880	1.1859870	0.0509660
C	3.1853440	1.7369710	0.7721460
C	4.3833700	1.0580530	0.9553800
C	4.5591660	-0.2317080	0.4239070
C	3.4916960	-0.7974010	-0.2884820
C	2.2565290	-0.1639870	-0.4714920
C	1.2560180	-0.9168150	-1.3346810
C	-0.1039180	-1.0745540	-0.9632940
C	-0.7392830	-0.6671530	0.3006060
C	-2.0897560	-0.0056690	0.0813090
C	-2.1607520	1.3950230	-0.0549810
C	-3.3822270	2.0204840	-0.3049660
C	-4.5631320	1.2689970	-0.4298610
C	-4.4990920	-0.1215240	-0.3034350
C	-3.2741910	-0.7520140	-0.0450270
H	3.0485430	2.7416300	1.1721440

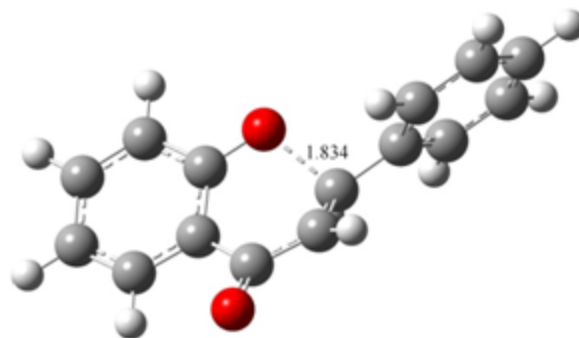
H	5.1924860	1.5335870	1.5162010
H	5.4923290	-0.7772080	0.5591490
H	3.6091740	-1.7811250	-0.7399560
H	-0.7383420	-1.5788840	-1.6898430
H	-0.0995030	-0.0055170	0.8873830
H	-1.2261590	1.9514770	0.0053120
H	-3.4177100	3.1040470	-0.4108010
H	-5.5142440	1.7624930	-0.6252060
H	-5.4044680	-0.7199800	-0.4035640
H	-3.2167480	-1.8342050	0.0450690
O	1.6983510	-1.4239450	-2.4146000
O	0.9901840	1.8781120	-0.1053470
O	-0.8616040	-1.9525250	0.9542160
O	-1.5240620	-1.8137390	2.4607430
H	-2.4064750	-1.5076730	2.1954410



TS-A1

Symbol	X	Y	Z
C	-1.9192430	-0.9285690	0.5430510
C	-3.0021810	-1.8831310	0.5845730
C	-4.2486400	-1.6232520	0.0512240

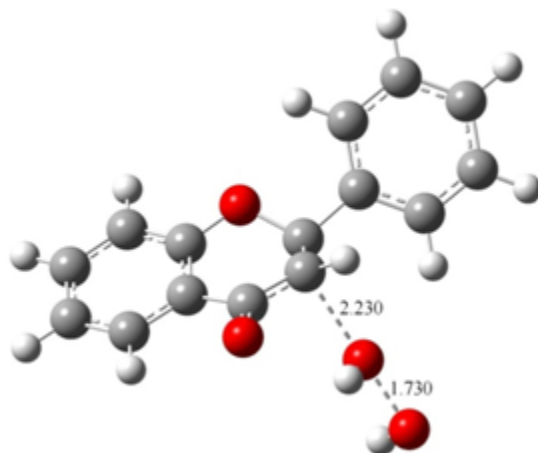
C	-4.5223260	-0.3854500	-0.5716260
C	-3.5160490	0.5667550	-0.6215780
C	-2.2247100	0.3444900	-0.0892400
C	-1.2885410	1.5080730	-0.1574740
C	0.1740880	1.3502700	0.5274290
C	0.7701540	0.1659470	-0.1631210
C	2.1740470	-0.1215130	-0.2209590
C	3.1705140	0.7718230	0.2561030
C	4.5055760	0.3726720	0.2870000
C	4.8859590	-0.8901470	-0.1823340
C	3.9164890	-1.7731100	-0.6824190
C	2.5809170	-1.3919930	-0.7089070
H	-2.7833440	-2.8322210	1.0670930
H	-5.0266930	-2.3840910	0.1094740
H	-5.4994450	-0.1830550	-1.0024160
H	-3.6975440	1.5349520	-1.0795560
H	-0.1583420	0.9027870	1.5019650
H	0.1489810	-0.4672770	-0.7837440
H	2.8286980	1.7570470	0.5637500
H	5.2611790	1.0599030	0.6596930
H	5.9333390	-1.1828940	-0.1741560
H	4.2093210	-2.7539840	-1.0479990
H	1.8212880	-2.0808770	-1.0681830
O	-0.7800440	-1.2459410	1.0469150
O	-1.5990400	2.5715250	-0.6637690
O	0.9073650	2.4409810	0.6348220



TS-B1

Symbol	X	Y	Z
C	-1.5861110	-0.3925680	-0.5746280
C	-2.5645190	-1.2149150	-1.1975220
C	-3.9193360	-1.0772360	-0.9142530
C	-4.3673800	-0.0845240	-0.0283960
C	-3.4278780	0.7798810	0.5331150
C	-2.0532830	0.6641020	0.2836410
C	-1.1401120	1.7871450	0.7246620
C	0.2525580	1.5022590	0.6374170
C	0.6626950	0.1569280	0.5234300
C	2.0778710	-0.1641470	0.2010670
C	2.7783280	0.5459130	-0.7890380
C	4.1087800	0.2432920	-1.0811480
C	4.7683470	-0.7827740	-0.3942340
C	4.0784140	-1.5078940	0.5821350
C	2.7447530	-1.2046970	0.8669410
H	-2.2107580	-1.9853600	-1.8778450
H	-4.6333780	-1.7532970	-1.3831080
H	-5.4261190	0.0249490	0.1942670
H	-3.7382650	1.6084480	1.1648830

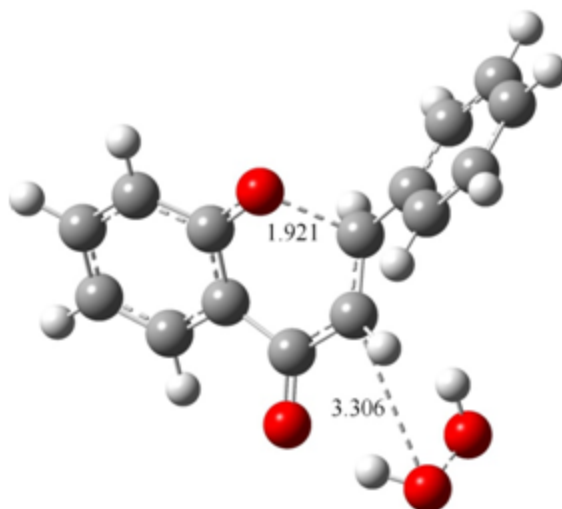
H	0.9522560	2.3219780	0.5075870
H	0.2239510	-0.5649700	1.2148750
H	2.2590740	1.3278790	-1.3340900
H	4.6320140	0.8032280	-1.8528380
H	5.8041430	-1.0201950	-0.6246810
H	4.5767130	-2.3128360	1.1174720
H	2.2069100	-1.7776900	1.6184050
O	-0.3094700	-0.6455060	-0.8179050
O	-1.6329070	2.9124950	0.9914530



TS-B2

Symbol	X	Y	Z
C	1.6798260	-1.1276260	-0.2224090
C	2.5134910	-2.1107220	-0.7730990
C	3.8949650	-1.9117650	-0.8020330
C	4.4520510	-0.7391890	-0.2742560
C	3.6152950	0.2220820	0.2952120
C	2.2261250	0.0499260	0.3310810
C	1.3367260	1.0102660	1.0740260

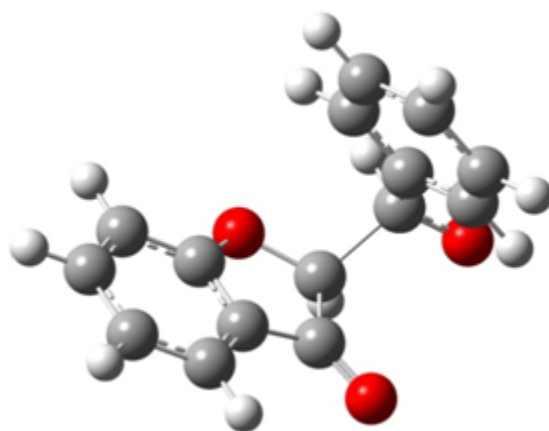
C	-0.0438450	0.8299870	0.8399410
C	-0.4841570	-0.1627340	-0.1998990
C	-1.9367540	-0.5670560	-0.0648500
C	-2.9224940	0.4152460	-0.2600690
C	-4.2750910	0.0914880	-0.1401490
C	-4.6663160	-1.2158680	0.1728460
C	-3.6889490	-2.1948400	0.3660940
C	-2.3317650	-1.8727700	0.2480530
H	2.0620160	-3.0115400	-1.1788020
H	4.5360100	-2.6720910	-1.2426670
H	5.5280270	-0.5854530	-0.2984200
H	4.0113820	1.1239550	0.7531770
H	-0.7610150	1.2022930	1.5608430
H	-0.3438400	0.2641180	-1.2076210
H	-2.6118090	1.4308490	-0.4923370
H	-5.0258240	0.8634200	-0.2914670
H	-5.7205100	-1.4664330	0.2648240
H	-3.9797480	-3.2140070	0.6109770
H	-1.5713770	-2.6313360	0.3973060
O	0.3383730	-1.3755090	-0.2005860
O	1.8525740	1.8595650	1.8526000
O	-0.4514150	2.6299950	-0.4130530
H	0.1003860	3.0883320	0.2404750
O	-0.7610670	4.0768200	-1.3102770
H	-0.2660600	3.7823820	-2.0886990



TS-C1

Symbol	X	Y	Z
C	-1.4871260	-1.5143370	-0.1767020
C	-2.3501620	-2.6480710	-0.2479040
C	-3.7127260	-2.5455420	-0.0074090
C	-4.3047290	-1.2994170	0.2671860
C	-3.4985620	-0.1663600	0.2571670
C	-2.1115980	-0.2283460	0.0342120
C	-1.3789520	1.0466370	-0.2222490
C	0.0506970	0.9786270	-0.2366540
C	0.6728260	-0.1280210	0.3597930
C	2.1137740	-0.4166110	0.1678550
C	2.8521010	-1.0161490	1.2007230
C	4.2116250	-1.2965350	1.0473070
C	4.8565840	-0.9928320	-0.1548470
C	4.1282020	-0.4117660	-1.1993580
C	2.7713820	-0.1306810	-1.0405910
H	-1.8881480	-3.6098000	-0.4537450

H	-4.3255350	-3.4457430	-0.0275820
H	-5.3718700	-1.2207590	0.4573250
H	-3.9269800	0.8225700	0.3957690
H	0.5856850	1.6330660	-0.9194190
H	0.3011210	-0.4473190	1.3312190
H	2.3488580	-1.2639040	2.1318050
H	4.7650500	-1.7556160	1.8627260
H	5.9136070	-1.2133750	-0.2807600
H	4.6187300	-0.1832100	-2.1422080
H	2.2052550	0.3005700	-1.8597880
O	-2.0327700	2.0826850	-0.5434590
O	-0.1950800	-1.7073390	-0.3058100
O	-0.4673140	4.2436320	-0.3216920
H	-1.1505530	3.5189220	-0.4457780
O	0.0301350	3.9379060	1.0165770
H	0.3649820	3.0259530	0.8943290

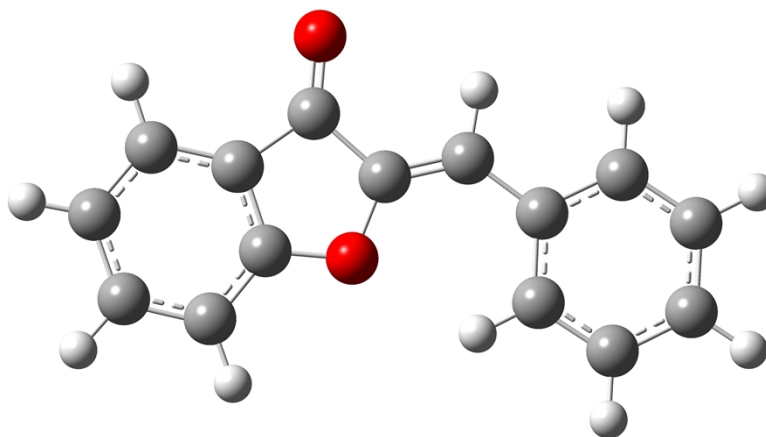


TS-D1

Symbol	X	Y	Z
C	0.3026580	0.1872560	0.3921480

C	0.3329170	-0.2388400	1.7518140
C	1.3517920	-1.0796830	2.1810680
C	2.3687820	-1.5289620	1.3086840
C	2.3512040	-1.1179150	-0.0214340
C	1.3279730	-0.2767480	-0.4753980
C	1.1991870	0.2514900	-1.8403880
C	-0.0981370	1.0444820	-2.0075270
C	-0.0750760	2.4337670	-2.5435590
C	-1.2958950	3.3103260	-2.2667050
C	-1.5335030	3.8818630	-1.0081810
C	-2.6392020	4.7093420	-0.8011000
C	-3.5207950	4.9855020	-1.8545530
C	-3.2873810	4.4200660	-3.1116200
C	-2.1821270	3.5854250	-3.3135830
H	-0.4429210	0.1046520	2.4304190
H	1.3673720	-1.4014270	3.2213770
H	3.1514880	-2.1869090	1.6762140
H	3.1161020	-1.4347060	-0.7263360
H	-1.0011140	0.4973430	-2.2469250
H	0.8270090	2.9875100	-2.2028950
H	-0.8619490	3.6488500	-0.1863750
H	-2.8185040	5.1365390	0.1834510
H	-4.3807640	5.6321030	-1.6936510
H	-3.9670180	4.6289890	-3.9356370
H	-1.9730020	3.1276260	-4.2764250
O	0.0207930	1.8822540	-3.7885570
O	2.0353680	0.0835690	-2.7223640

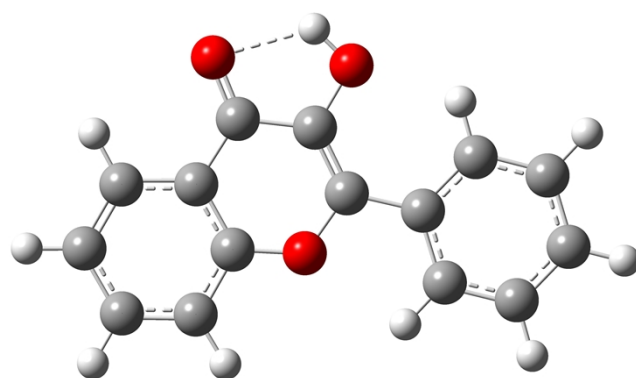
O -0.5932330 0.9788570 -0.1176560



Aurone

Symbol	X	Y	Z
C	-2.48145800	0.56868500	-0.00028300
C	-1.91540100	-0.70898400	-0.00014500
C	-2.67986700	-1.86879700	-0.00014800
C	-4.06835300	-1.69972600	-0.00029900
C	-4.66213200	-0.42360400	-0.00044000
C	-3.87051800	0.72451800	-0.00043300
C	-1.36420400	1.52795600	-0.00023100
H	-2.22035000	-2.85109400	-0.00003900
H	-4.70436900	-2.58016300	-0.00030700
H	-5.74406900	-0.33816800	-0.00055400
H	-4.30682400	1.71859200	-0.00054000
O	-0.53640700	-0.68177000	-0.00000800

O	-1.38372000	2.75315700	-0.00031000
C	-0.14902700	0.65418400	-0.00005500
C	1.12843100	1.08318900	0.00004500
H	1.20255800	2.16893700	-0.00001700
C	2.38288400	0.34334600	0.00021600
C	3.58576400	1.08199000	0.00028100
C	2.46383600	-1.06684200	0.00032000
C	4.82313700	0.44228500	0.00044400
H	3.53920000	2.16775200	0.00020300
C	3.70407200	-1.70182000	0.00048300
H	1.55539400	-1.65587800	0.00027400
C	4.88696700	-0.95440700	0.00054500
H	5.73572200	1.03102300	0.00049100
H	3.74914300	-2.78709300	0.00056200
H	5.84982500	-1.45684600	0.00067200



Product

Symbol	X	Y	Z
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C	-4.36985300	-0.85324900	-0.00027800
C	-3.67600500	0.34552700	-0.00007700
C	-2.26640300	0.34956900	0.00001400
C	-1.58294100	-0.87657600	-0.00012700
C	-2.27724200	-2.09475300	-0.00033000
C	-3.66476500	-2.07394100	-0.00040000
H	-5.45512200	-0.85614500	-0.00033900
H	-4.18763500	1.30232800	0.00002900
C	-1.48392700	1.57788400	0.00025100
H	-1.71893900	-3.02475000	-0.00044000
H	-4.21090700	-3.01245200	-0.00056100
C	0.56695800	0.18104700	0.00003500
C	-0.03298100	1.41379000	0.00019900
C	1.99966100	-0.14421400	0.00005900
C	2.99098100	0.85986700	-0.00017300
C	2.41096500	-1.49414400	0.00029900
C	4.34255800	0.51591700	-0.00017500
H	2.70330300	1.90172100	-0.00035700
C	3.76363200	-1.82612200	0.00030400
H	1.66672200	-2.28065600	0.00048100
C	4.73793400	-0.82368200	0.00006600
H	5.08957000	1.30423300	-0.00036500
H	4.05697900	-2.87188200	0.00049800

H	5.79220800	-1.08441600	0.00006900
O	0.65536300	2.58107600	0.00041100
H	-0.04699000	3.26860500	0.00061700
O	-0.22425000	-0.94361800	-0.00011100
O	-1.95201600	2.73097400	0.00012800