

Analysis of Conformational, Structural, Magnetic, and Electronic Properties
Related to Antioxidant Activity: Revisiting Flavan, Anthocyanidin, Flavanone,
Flavonol, Isoflavone, Flavone, and Flavan-3-ol

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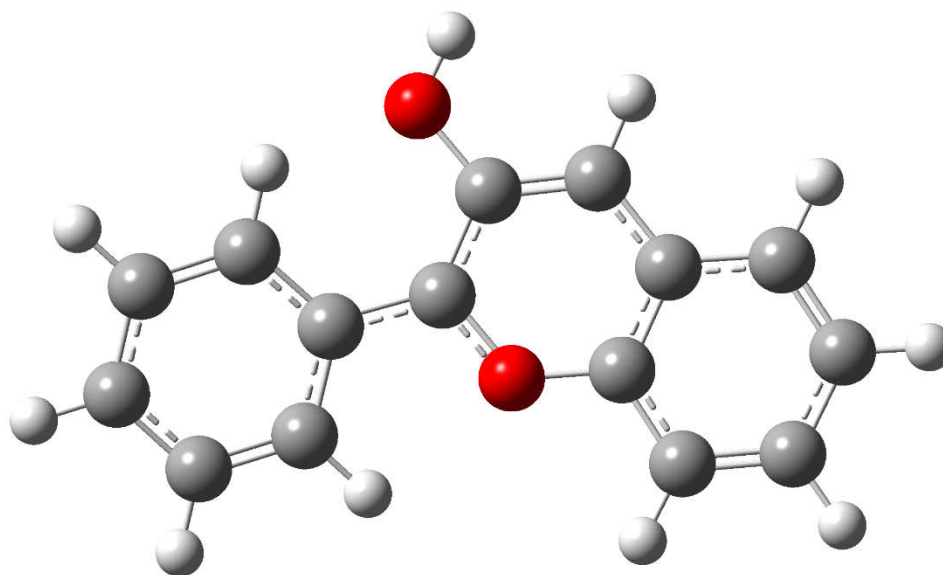
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ANTHOCYANIDIN



Nuclear charges R N= 28

8.00000000E+00 8.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
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6.00000000E+00 6.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00
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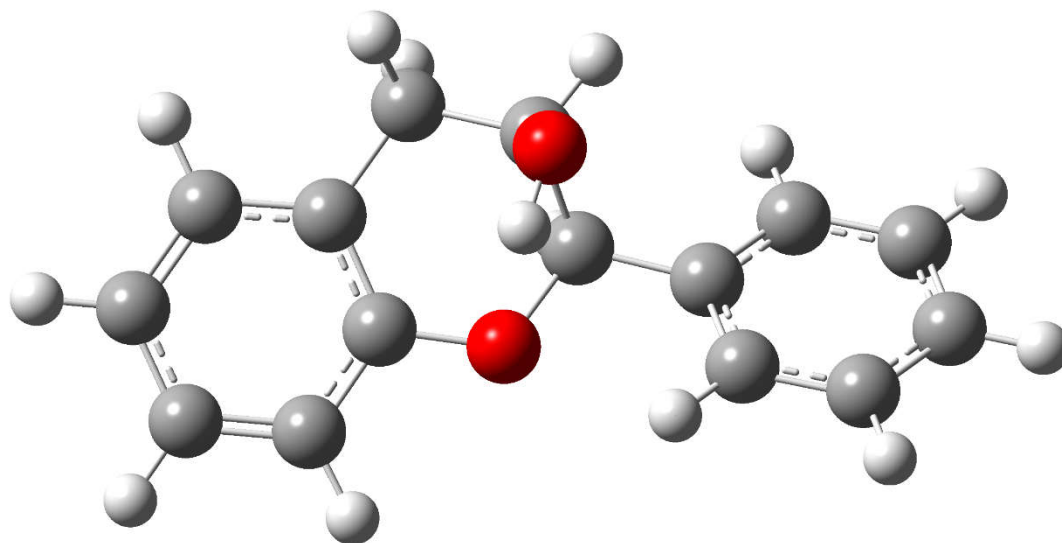
Current cartesian coordinates R N= 84

7.30362839E-01 -1.36837613E+00 8.30593685E-02 -1.47629929E+00 5.02475939E+00
-2.40457706E-01 4.41069434E+00 1.23546083E+00 -4.16996402E-02 -8.96161241E-01
5.78241874E-01 -3.83226547E-03 3.32313660E+00 -1.17229078E+00 6.88971446E-02
-3.51555556E+00 -1.48086629E-01 -2.09455697E-03 1.82110545E-01 3.03705604E+00
-1.22129424E-01 2.75144054E+00 3.32878410E+00 -1.13874736E-01 7.07112547E+00
1.40545048E+00 -3.75844000E-02 4.73968496E+00 -3.37629868E+00 1.58874518E-01
-4.12704871E+00 -2.71785982E+00 -3.77037551E-01 -5.48224977E+00 1.60164551E+00
3.95047955E-01 8.49731924E+00 -7.57608660E-01 5.29807755E-02 7.33241765E+00
-3.14812300E+00 1.53777101E-01 -6.61100315E+00 -3.49539277E+00 -3.61463010E-01
-7.96531583E+00 7.86725146E-01 4.21807359E-01 -8.53884722E+00 -1.74616238E+00

4.12555515E-02 3.54969181E+00 5.20979919E+00 -2.06068515E-01 7.95853887E+00
3.24182167E+00 -1.15308281E-01 3.80765458E+00 -5.18636139E+00 2.39842054E-01
-2.64334660E+00 -4.07635758E+00 -6.90305015E-01 -5.05892026E+00 3.56580137E+00
6.81075230E-01 1.05324376E+01 -6.36775499E-01 5.20504348E-02 8.48955411E+00
-4.82582308E+00 2.26423082E-01 -7.06175849E+00 -5.46065711E+00 -6.65930394E-01
-9.46076979E+00 2.13582534E+00 7.40139961E-01 -1.04840355E+01 -2.36322240E+00
Total Energy R -7.280515838049453E+02

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FLAVAN-3-OL_CONFORMER



Nuclear charges R N= 31

8.00000000E+00 8.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00
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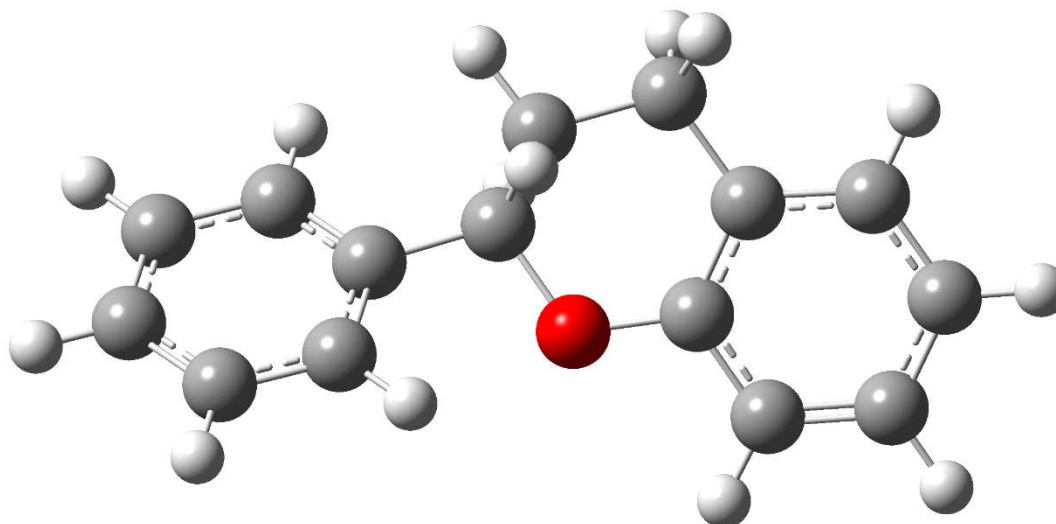
Current cartesian coordinates R N= 93

-6.52754733E-01 -1.51176606E+00 -1.75713373E-01 3.23558339E-01 2.44090996E+00
3.27252976E+00 6.39089952E-02 2.93128992E+00 5.98388847E-01 9.06830578E-01
6.24639639E-01 -9.45704577E-01 -2.65579501E+00 3.59047316E+00 -9.64230960E-02
-4.32355227E+00 1.27561374E+00 -2.07672884E-01 3.64068854E+00 -7.30532580E-02
-5.95764077E-01 -3.27152943E+00 -1.13495348E+00 -2.70098358E-01 -6.95091632E+00
1.46703296E+00 -2.38178652E-01 -4.76627156E+00 -3.28941305E+00 -3.32696575E-01
4.38247603E+00 -2.02537225E+00 9.95927418E-01 5.47788543E+00 1.31279278E+00
-1.87380650E+00 -8.47310085E+00 -6.62789833E-01 -3.17505276E-01 -7.37116651E+00
-3.05134717E+00 -3.57816397E-01 6.93054444E+00 -2.57115452E+00 1.31690969E+00
8.02269143E+00 7.72473547E-01 -1.54937412E+00 8.75625383E+00 -1.17324753E+00
5.42060376E-02 1.31004188E+00 4.51872862E+00 2.21426024E-01 5.39645626E-01
1.01242091E+00 -2.94216255E+00 -2.66816183E+00 4.55541736E+00 -1.92375764E+00
-3.37644029E+00 4.92262824E+00 1.29718507E+00 -7.80208613E+00 3.32542625E+00
-1.80951923E-01 -3.85219722E+00 -5.11258081E+00 -3.69575766E-01 -2.18486524E-01
7.23029192E-01 3.66837046E+00 2.96035533E+00 -3.12875511E+00 1.95072030E+00
4.91859139E+00 2.81745905E+00 -3.14263104E+00 -1.05045487E+01 -4.67967095E-01
-3.37656260E-01 -8.54148748E+00 -4.72292989E+00 -4.11957900E-01 7.48867580E+00
-4.09385591E+00 2.55791189E+00 9.42955563E+00 1.86129086E+00 -2.55191942E+00

Total Energy R -7.301074581668781E+02

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FLAVAN



Nuclear charges R N= 30

8.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00
1.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00
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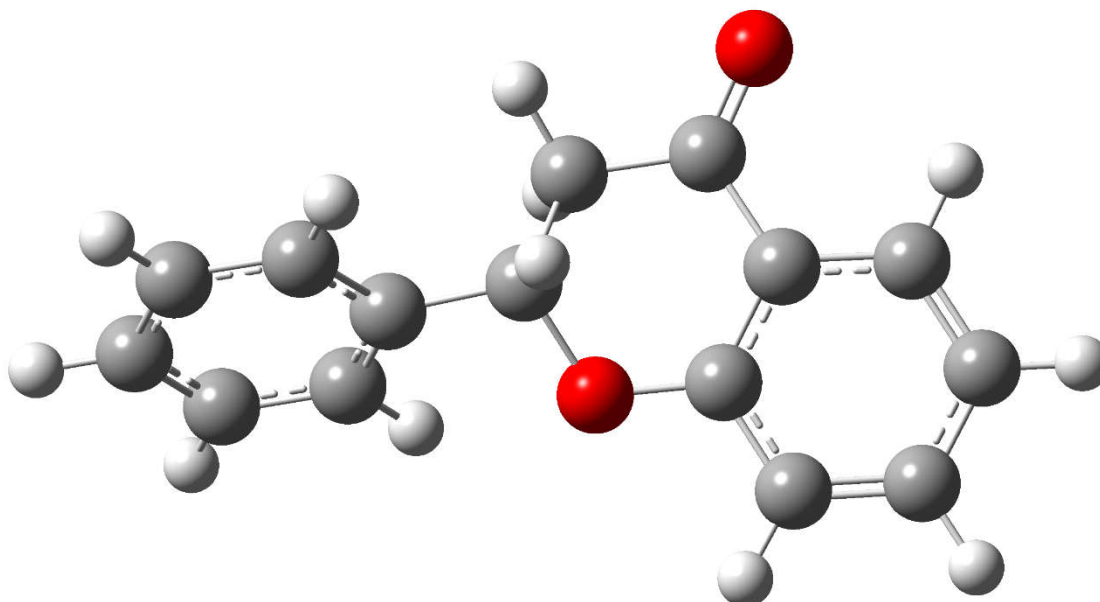
Current cartesian coordinates R N= 90

6.22460455E-01 -1.26893569E+00 -5.87430130E-01 -9.55177489E-01 9.84102109E-01
-7.49286359E-01 -8.28278974E-02 2.92183856E+00 1.20740304E+00 2.64758445E+00
3.69645390E+00 6.74245739E-01 4.29896136E+00 1.40852349E+00 2.38977732E-01
-3.66153232E+00 1.81425323E-01 -3.94131048E-01 3.22342405E+00 -9.19967363E-01
-3.60602230E-01 6.92207078E+00 1.53681385E+00 4.49070450E-01 4.71053019E+00
-3.05546022E+00 -7.17046814E-01 -4.28861593E+00 -1.79306524E+00 1.22509970E+00
-5.58175111E+00 1.49612382E+00 -1.62099222E+00 8.43053978E+00 -5.72858877E-01
8.31914006E-02 7.31050365E+00 -2.88118190E+00 -4.98644963E-01 -6.80332885E+00
-2.43229717E+00 1.61759165E+00 -8.09735865E+00 8.63699476E-01 -1.22293125E+00

-8.71403163E+00 -1.10360063E+00 4.01580763E-01 -7.19092244E-01 1.78292145E+00
-2.64238798E+00 -2.46199011E-01 2.06937291E+00 3.07809882E+00 -1.33764854E+00
4.55282575E+00 1.15847804E+00 3.39380308E+00 4.80333057E+00 2.24403612E+00
2.70115148E+00 4.92633691E+00 -9.86352214E-01 7.78148098E+00 3.33108304E+00
9.24654491E-01 3.78635473E+00 -4.81661237E+00 -1.17022815E+00 -2.79555885E+00
-2.84110729E+00 2.13656196E+00 -5.10857978E+00 3.01455375E+00 -2.90749878E+00
1.04589023E+01 -4.25888302E-01 2.55946411E-01 8.46423216E+00 -4.54185138E+00
-7.80567809E-01 -7.27213752E+00 -3.97617039E+00 2.86966132E+00 -9.57095006E+00
1.89529064E+00 -2.18987147E+00 -1.06693847E+01 -1.60589453E+00 7.07756622E-01
Total Energy R -6.549070362674269E+02

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FLAVANONE



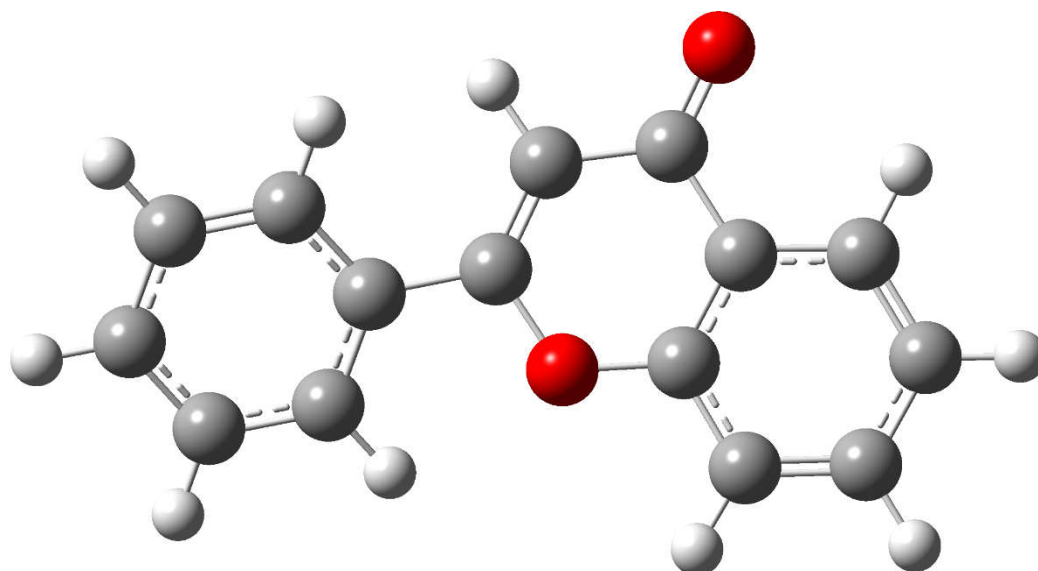
Nuclear charges R N= 29

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6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
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6.00000000E+00 6.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00

1.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00
Current cartesian coordinates R N= 87
3.60311566E-01 -1.71531503E+00 1.33659294E-01 3.58848235E+00 5.30677339E+00
-7.19727370E-01 -1.08541575E+00 5.56847405E-01 7.71039911E-01 -1.68596362E-01
2.76141659E+00 -8.46800083E-01 -3.84473294E+00 -1.79737259E-02 4.12112646E-01
2.63527722E+00 3.17833634E+00 -5.36458478E-01 4.14938041E+00 8.88515829E-01
-8.84993266E-02 2.96438142E+00 -1.45875562E+00 1.57514748E-01 -5.62072869E+00
1.04196511E+00 2.03601530E+00 -4.65852151E+00 -1.52283796E+00 -1.58547129E+00
6.78788662E+00 1.00244802E+00 -3.33319064E-02 4.38229061E+00 -3.65592783E+00
4.01927416E-01 8.20830159E+00 -1.16961694E+00 2.27305958E-01 6.99067400E+00
-3.50259753E+00 4.35372457E-01 -8.18421560E+00 6.24322260E-01 1.65838014E+00
-7.21990541E+00 -1.95043778E+00 -1.95557253E+00 -8.98868708E+00 -8.73675595E-01
-3.40173642E-01 -7.16316687E-01 9.74496130E-01 2.76170887E+00 -1.16687315E+00
4.49116115E+00 -3.63721816E-01 -5.57751579E-01 2.34867488E+00 -2.83351369E+00
-5.00052156E+00 2.19183717E+00 3.60941831E+00 -3.27780454E+00 -2.38297241E+00
-2.81639630E+00 7.66667891E+00 2.83454070E+00 -2.28662406E-01 3.40531708E+00
-5.43611038E+00 5.84759190E-01 1.02453361E+01 -1.07048325E+00 2.64440542E-01
8.09317929E+00 -5.20981581E+00 6.33950438E-01 -9.54757416E+00 1.45559538E+00
2.93082131E+00 -7.83694407E+00 -3.13191730E+00 -3.50249587E+00 -1.09814082E+01
Total Energy R -7.289099688511744E+02

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FLAVONE



Nuclear charges R N= 27

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8.00000000E+00 8.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00
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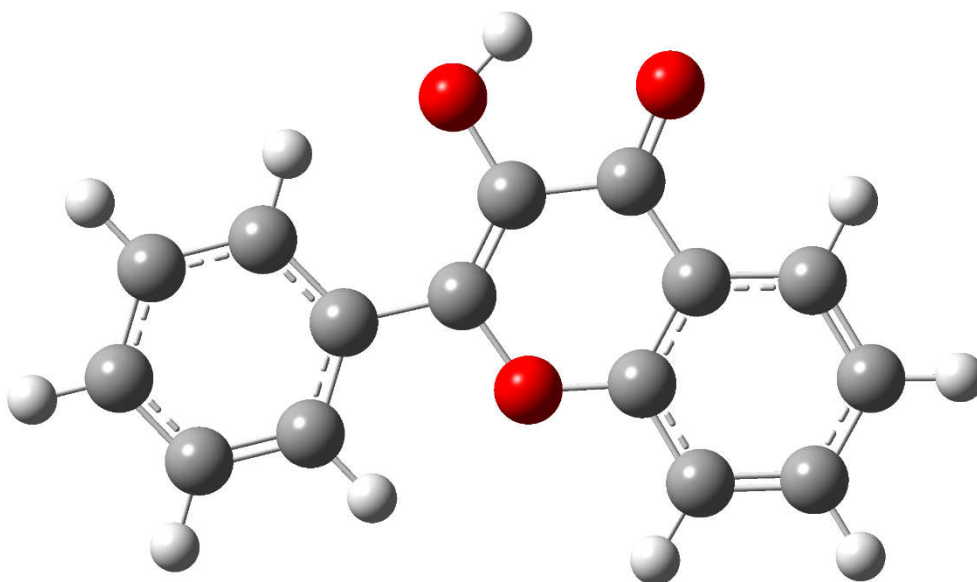
Current cartesian coordinates R N= 81

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-4.19462508E-01 4.17132854E+00 9.17856986E-01 -5.83490735E-02 -1.11607225E+00
6.23836388E-01 -3.03773475E-02 2.93852601E+00 -1.39384120E+00 1.31927450E-01
-3.84363680E+00 8.45898105E-02 5.27611534E-03 2.68447123E+00 3.26014417E+00
-2.51127594E-01 -3.19684968E-02 2.91250259E+00 -2.52624258E-01 6.81164254E+00
9.44955659E-01 -6.79791179E-02 4.26043668E+00 -3.65390451E+00 3.18496331E-01
-5.57565772E+00 1.94845881E+00 7.03648971E-01 -4.73202917E+00 -2.30533359E+00
-6.70544749E-01 8.15405106E+00 -1.28227555E+00 1.12862003E-01 6.86918659E+00
-3.58499754E+00 3.06101617E-01 -8.14460432E+00 1.43907180E+00 6.96764699E-01
-7.30417131E+00 -2.80686124E+00 -6.76682579E-01 -9.01750095E+00 -9.38369963E-01
2.71742617E-03 -1.17504682E+00 4.58149737E+00 -4.67516353E-01 7.74149929E+00
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2.75514888E+00 -2.19017368E-01 3.22569069E+00 -5.40394397E+00 4.70585269E-01
-4.91686895E+00 3.78899915E+00 1.28788993E+00 -3.39892377E+00 -3.75496140E+00
-1.19296709E+00 1.01939235E+01 -1.25433217E+00 1.05783089E-01 7.92201159E+00
-5.32783336E+00 4.49749148E-01 -9.46540383E+00 2.89443870E+00 1.24805072E+00
-7.97143360E+00 -4.66009108E+00 -1.21289048E+00 -1.10204217E+01 -1.33301470E+00
Total Energy R -7.277066172437681E+02

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FLAVONOL_NEUTRAL

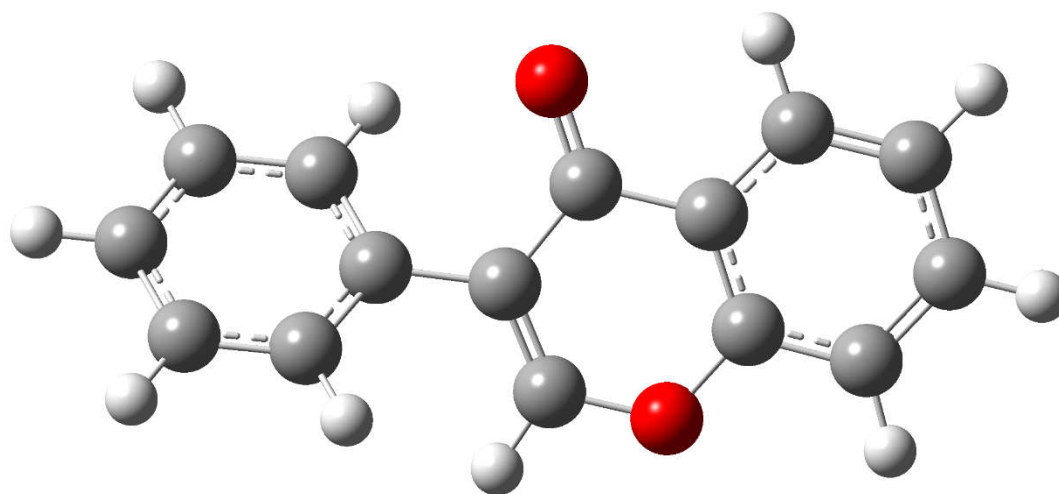


Nuclear charges R N= 28
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6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 1.00000000E+00 1.00000000E+00
1.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00
Current cartesian coordinates R N= 84
4.29208643E-01 -1.81382639E+00 -1.92376946E-05 -1.28795918E+00 4.86016711E+00

-7.92917698E-04 3.67127457E+00 5.14035591E+00 -5.30252532E-05 4.26925814E+00
6.45580501E-01 4.82215346E-04 -1.07986045E+00 3.32663553E-01 -1.31657266E-04
3.02656530E+00 -1.67192767E+00 -1.97180790E-05 -3.78049882E+00 -2.76261064E-01
-1.10530874E-05 5.04781118E-02 2.62700720E+00 -4.79338530E-04 2.77522761E+00
2.93995871E+00 -6.74486418E-07 6.91588394E+00 6.81339678E-01 3.59710826E-04
4.35742733E+00 -3.94026332E+00 -1.57410473E-05 -4.54530310E+00 -2.81097305E+00
-5.56073478E-04 -5.63204638E+00 1.61478725E+00 6.34555222E-04 8.25226137E+00
-1.55023934E+00 2.33569066E-04 6.96159595E+00 -3.86464780E+00 9.03781355E-06
-7.08643417E+00 -3.43368275E+00 -4.29991936E-04 -8.17324643E+00 9.69478732E-01
7.78699317E-04 -8.91331518E+00 -1.54655194E+00 2.48461169E-04 7.84890151E+00
2.49592686E+00 4.96010465E-04 3.32566683E+00 -5.69826825E+00 -1.92059525E-04
-3.13673909E+00 -4.28055017E+00 -1.06034503E-03 -5.07276229E+00 3.56919670E+00
9.84552944E-04 1.02918325E+01 -1.52627356E+00 2.00558629E-04 8.01678622E+00
-5.61183911E+00 -6.70048978E-05 -7.64310135E+00 -5.39802741E+00 -8.66498927E-04
-9.57951948E+00 2.44945588E+00 1.30213690E-03 -1.08955943E+01 -2.03592579E+00
Total Energy R -8.029129135942353E+02

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ISOFLAVONE



Nuclear charges R N= 27

8.00000000E+00 8.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00
6.00000000E+00 6.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00
1.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00

Current cartesian coordinates R N= 81

2.50013259E+00 -3.48371521E+00 -6.89538007E-01 2.57420531E-02 3.74365795E+00
5.52192039E-01 -9.81350472E-01 -6.00557958E-01 -1.64285390E-01 3.46447829E+00
8.92187182E-01 1.51746779E-01 7.57916183E-01 1.53269586E+00 2.08502667E-01
4.24850059E+00 -1.57580162E+00 -2.86077478E-01 -3.75588912E+00 -2.47560366E-01
-4.86643809E-02 -2.02274094E-02 -2.90811369E+00 -6.13925434E-01 5.31143924E+00
2.74485491E+00 5.39301368E-01 6.78753038E+00 -2.23945372E+00 -3.52545997E-01
-5.26121364E+00 -1.97704949E+00 1.25765572E+00 -4.92369941E+00 1.78252943E+00
-1.26546064E+00 7.83979811E+00 2.12043895E+00 4.83367676E-01 8.57551736E+00
-3.81162845E-01 3.49486626E-02 -7.87074039E+00 -1.71546833E+00 1.31244289E+00
-7.53069332E+00 2.04373038E+00 -1.20392944E+00 -9.01414115E+00 2.95253645E-01
7.61051986E-02 -1.14523682E+00 -4.56302640E+00 -9.80386674E-01 4.68270743E+00

4.65590135E+00 8.78702665E-01 7.29795792E+00 -4.18168204E+00 -7.03726490E-01
-4.38114906E+00 -3.51400856E+00 2.27658044E+00 -3.78380423E+00 3.16758517E+00
-2.23015772E+00 9.25680219E+00 3.55680252E+00 7.84460562E-01 1.05578245E+01
-8.65507234E-01 -9.42740341E-03 -9.00444348E+00 -3.06881448E+00 2.33868377E+00
-8.40695297E+00 3.62386523E+00 -2.15499114E+00 -1.10440540E+01 5.10208543E-01
Total Energy R -7.276995241295074E+02
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