Supplemental data

Semiexperimental equilibrium structure of 1-methylisatin from gas-phase electron diffraction data and structural changes in isatin due to 1-methyl and 5-fluoro substituents as predicted by coupled cluster computations

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Figure S1. Molecular model of 1-methylisatin with atom numbering (according to the used Z-matrix)
Table S1. Optimized Cartesian coordinates of 1-methylisatin, Å.

| At  | x       | y       | z       | x       | y       | z       |
|-----|---------|---------|---------|---------|---------|---------|
| C1  | 0.000000| 0.000000| 0.000000| 0.000000| 0.000000| 0.000000|
| C2  | 0.000000| 1.397658| 0.000000| 0.000000| 1.400595| 0.000000|
| N3  | 1.302421| 1.901167| 0.000000| 1.304786| 1.905205| 0.000000|
| C4  | 2.229662| 0.885488| 0.000000| 2.234161| 0.888100| 0.000000|
| C5  | 1.403368| −0.430636| 0.000000| 1.406401| −0.431301| 0.000000|
| C6  | −1.184596| 2.108796| 0.000000| −1.186892| 2.113555| 0.000000|
| C7  | −2.373781| 1.379456| 0.000000| −2.378544| 1.382725| 0.000000|
| C8  | −2.378388| −0.011950| 0.000000| −2.383298| −0.011570| 0.000000|
| C9  | −1.179380| −0.718048| 0.000000| −1.181976| −0.719412| 0.000000|
| O10 | 3.433634| 0.999449| 0.000000| 3.439961| 1.003051| 0.000000|
| O11 | 1.878046| −1.541952| 0.000000| 1.882232| −1.544214| 0.000000|
| C12 | 1.641610| 3.297845| 0.000000| 1.644056| 3.304782| 0.000000|
| H13 | −1.198035| 3.188156| 0.000000| −1.200279| 3.194236| 0.000000|
| H14 | −3.313320| 1.912255| 0.000000| −3.319176| 1.916293| 0.000000|
| H15 | −3.318444| −0.541731| 0.000000| −3.324619| −0.541815| 0.000000|
| H16 | −1.155114| −1.798077| 0.000000| −1.157985| −1.800740| 0.000000|
| H17 | 2.724121| 3.365931| 0.000000| 2.727917| 3.372714| 0.000000|
| H18 | 1.248747| 3.790964| 0.886628| 1.250049| 3.797757| 0.887895|
| H19 | 1.248747| 3.790964| −0.886628| 1.250049| 3.797757| −0.887895|

(to be continued)
| At   | x  | y  | z  |     | x  | y  | z  |
|------|----|----|----|-----|----|----|----|
| C1   | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| C2   | 0.00000 | 1.406272 | 0.00000 | 0.00000 | 1.401000 | 0.00000 | 0.00000 |
| N3   | 1.309976 | 1.909579 | 0.00000 | 1.307013 | 1.902715 | 0.00000 | 0.00000 |
| C4   | 2.241551 | 0.886773 | 0.00000 | 2.234424 | 0.883503 | 0.00000 | 0.00000 |
| C5   | 1.410397 | -0.437382 | 0.00000 | 1.405973 | -0.437160 | 0.00000 | 0.00000 |
| C6   | -1.189117 | 2.125310 | 0.00000 | -1.183824 | 2.117949 | 0.00000 | 0.00000 |
| C7   | -2.385453 | 1.390654 | 0.00000 | -2.375390 | 1.384893 | 0.00000 | 0.00000 |
| C8   | -2.395630 | -0.008964 | 0.00000 | -2.385122 | -0.009073 | 0.00000 | 0.00000 |
| C9   | -1.188763 | -0.718674 | 0.00000 | -1.183149 | -0.717089 | 0.00000 | 0.00000 |
| O10  | 3.445755 | 1.002448 | 0.00000 | 3.434076 | 0.996904 | 0.00000 | 0.00000 |
| O11  | 1.886016 | -1.548811 | 0.00000 | 1.880280 | -1.543799 | 0.00000 | 0.00000 |
| C12  | 1.656790 | 3.314545 | 0.00000 | 1.650978 | 3.303091 | 0.00000 | 0.00000 |
| H13  | -1.200711 | 3.207420 | 0.00000 | -1.195134 | 3.197890 | 0.00000 | 0.00000 |
| H14  | -3.326879 | 1.926542 | 0.00000 | -3.315314 | 1.918844 | 0.00000 | 0.00000 |
| H15  | -3.338938 | -0.538842 | 0.00000 | -3.326957 | -0.537606 | 0.00000 | 0.00000 |
| H16  | -1.166731 | -1.801485 | 0.00000 | -1.160144 | -1.797844 | 0.00000 | 0.00000 |
| H17  | 2.743637 | 3.377604 | 0.00000 | 2.734952 | 3.369389 | 0.00000 | 0.00000 |
| H18  | 1.262995 | 3.810019 | 0.890445 | 1.256788 | 3.796653 | 0.888319 | 0.00000 |
| H19  | 1.262995 | 3.810019 | -0.890445 | 1.256788 | 3.796653 | -0.888319 | 0.00000 |

| At   | x  | y  | z  |     | x  | y  | z  |
|------|----|----|----|-----|----|----|----|
| B2PLYP/VTZ |  |  |  |     |  |  |  |
| C1   | -0.388100 | 0.671634 | 0.000005 | 0.00000 | 0.00000 | 0.00000 |
| C2   | -0.512531 | -0.726691 | 0.000006 | 1.40260 | 0.00000 | 0.00000 |
| N3   | 0.744654 | -1.342700 | 0.000006 | 1.91657 | 1.30374 | 0.00000 |
| C4   | 1.759716 | -0.404663 | 0.000004 | 0.91321 | 2.25032 | 0.00000 |
| C5   | 1.045889 | 0.986137 | 0.000004 | -0.40588 | 1.41712 | 0.00000 |
| C6   | -1.758943 | -1.330856 | 0.000006 | 2.12777 | -1.17986 | 0.00000 |
| C7   | -2.880414 | -0.496204 | 0.000005 | 1.40959 | -2.38232 | 0.00000 |
| C8   | -2.766290 | 0.893353 | 0.000004 | 0.01509 | -2.41951 | 0.00000 |
| C9   | -1.506243 | 1.488657 | 0.000003 | -0.67708 | -1.20741 | 0.00000 |
| O10  | 2.947467 | -0.624653 | 0.000002 | 1.06011 | 3.44692 | 0.00000 |
| O11  | 1.615679 | 2.049817 | 0.000003 | -1.51849 | 1.87723 | 0.00000 |
| C12  | 0.970613 | -2.769684 | 0.000007 | 3.32418 | 1.62273 | 0.00000 |
| H13  | -1.870030 | -2.404691 | 0.000007 | 3.21556 | -1.18412 | 0.00000 |
| H14  | -3.863419 | -0.945549 | 0.000005 | 1.95926 | -3.32102 | 0.00000 |
| H15  | -3.656271 | 1.504374 | 0.000003 | -0.49849 | -3.37843 | 0.00000 |
| H16  | -1.388172 | 2.562889 | 0.000002 | -1.76423 | -1.16999 | 0.00000 |
| H17  | 2.044875 | -2.927290 | 0.000007 | 3.40997 | 2.70513 | 0.00000 |
| H18  | 0.538182 | -3.231048 | 0.887568 | 3.81066 | 1.21964 | 0.88848 |
| H19  | 0.538182 | -3.231050 | -0.887553 | 3.81066 | 1.21964 | -0.88848 |

Note. Atom numbering is given in Fig. S1.
Table S2. Optimized Cartesian coordinates of isatin, Å.

| At  | MP2_AE/CVTZ | MP2_FC/CVTZ | MP2_FC/VQZ |
|-----|-------------|-------------|-------------|
|     | x    | y    | x    | y    | x    | y    |
| C1  | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| C2  | 0.000000 | 1.396784 | 0.000000 | 1.399707 | 0.000000 | 1.399126 |
| N3  | 1.308217 | 1.886374 | 1.310597 | 1.890256 | 1.310277 | 1.889765 |
| C4  | 2.239218 | 0.873184 | 2.243754 | 0.875703 | 2.242488 | 0.876765 |
| C5  | 1.400749 | -0.438919 | 1.403767 | -0.439620 | 1.403222 | -0.439195 |
| C6  | -1.185003 | 2.106009 | -1.187231 | 2.110826 | -1.185181 | 2.111149 |
| C7  | -2.373342 | 1.378547 | -2.378058 | 1.381909 | -2.376215 | 1.382697 |
| C8  | -2.378739 | -0.013986 | -2.383650 | -0.013516 | -2.382313 | -0.012175 |
| C9  | -1.181045 | -0.718663 | -1.183668 | -0.719984 | -1.183646 | -0.719508 |
| O10 | 3.440962 | 0.977590 | 3.447315 | 0.981206 | 3.444948 | 0.981731 |
| O11 | 1.868823 | -1.552869 | 1.872957 | -1.555189 | 1.873475 | -1.552630 |
| H12 | 1.561362 | 2.859100 | 1.563482 | 2.863991 | 1.563205 | 2.863194 |
| H13 | -1.197392 | 3.185902 | -1.199458 | 3.192039 | -1.197453 | 3.191896 |
| H14 | -3.312290 | 1.912216 | -3.318084 | 1.916371 | -3.315787 | 1.916952 |
| H15 | -3.318977 | -0.543320 | -3.325177 | -0.543272 | -3.323815 | -0.541014 |
| H16 | -1.155500 | -1.798589 | -1.158441 | -1.801209 | -1.159707 | -1.800828 |

| At  | MP2_FC/VTZ | CCSD(T)_FC/VTZ | CCSD(T)_AE/CVQZ |
|-----|-------------|----------------|----------------|
|     | x    | y    | x    | y    | x    | y    |
| C1  | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| C2  | 0.000000 | 1.401361 | 0.000000 | 1.397628 | 0.000000 | 1.392470 |
| N3  | 1.311685 | 1.891768 | 1.308517 | 1.884858 | 1.304727 | 1.887975 |
| C4  | 2.245331 | 0.875889 | 2.249712 | 0.867268 | 2.237198 | 0.865639 |
| C5  | 1.404909 | -0.439675 | 1.397879 | -0.443562 | 1.393182 | -0.442372 |
| C6  | -1.188421 | 2.113626 | -1.183273 | 2.112243 | -1.187453 | 2.104929 |
| C7  | -2.380694 | 1.384030 | -2.374338 | 1.383984 | -2.365148 | 1.379271 |
| C8  | -2.386427 | -0.013053 | -2.385449 | -0.011454 | -2.376409 | -0.011064 |
| C9  | -1.185176 | -0.720520 | -1.184660 | -0.715083 | -1.180289 | -0.712777 |
| O10 | 3.450469 | 0.981403 | 3.437953 | 0.972336 | 3.426088 | 0.969070 |
| O11 | 1.874800 | -1.556656 | 1.864788 | -1.554999 | 1.859328 | -1.548643 |
| H12 | 1.565143 | 2.855864 | 1.562573 | 2.855739 | 1.558509 | 2.848180 |
| H13 | -1.200621 | 3.194947 | -1.193218 | 3.189710 | -1.188001 | 3.180496 |
| H14 | -3.320858 | 1.918585 | -3.310444 | 1.918321 | -3.299585 | 1.912512 |
| H15 | -3.328190 | -0.542704 | -3.324109 | -0.538630 | -3.313516 | -0.537007 |
| H16 | -1.160343 | -1.801823 | -1.160048 | -1.792630 | -1.156437 | -1.788493 |
Table S3. Optimized Cartesian coordinates of 5-fluoroisatin, Å.

| At | MP2_AE/CVTZ | MP2_FC/CVTZ | MP2_FC/VQZ |
|----|-------------|-------------|-------------|
|    | x           | y           | x           | y           | x           | y           |
| C1 | 0.000000    | 0.000000    | 0.000000    | 0.000000    | 0.000000    | 0.000000    |
| C2 | 0.000000    | 1.396108    | 0.000000    | 1.399022    | 0.000000    | 1.398480    |
| N3 | 1.309373    | 1.886114    | 1.311774    | 1.889976    | 1.311388    | 1.889511    |
| C4 | 2.239757    | 0.873205    | 2.244305    | 0.875720    | 2.243058    | 0.876830    |
| C5 | 1.401715    | -0.439461   | 1.404746    | -0.440167   | 1.404259    | -0.439713   |
| C6 | -1.187751   | 2.101792    | -1.189969   | 2.106595    | -1.188257   | 2.107604    |
| C7 | -2.377062   | 1.377467    | -2.381879   | 1.380933    | -2.380164   | 1.383099    |
| C8 | -2.354957   | -0.009289   | -2.359618   | -0.008721   | -2.357143   | -0.005773   |
| C9 | -1.174718   | -0.729797   | -1.177262   | -0.731306   | -1.177391   | -0.730863   |
| O10| 3.441472    | 0.974909    | 3.447843    | 0.978492    | 3.445447    | 0.979120    |
| O11| 1.866100    | -1.554407   | 1.870226    | -1.556747   | 1.870722    | -1.554132   |
| H12| 1.562636    | 2.858716    | 1.564763    | 2.863588    | 1.564425    | 2.862824    |
| H13| -1.207227   | 3.181299    | -1.209319   | 3.187419    | -1.206383   | 3.187954    |
| H14| -3.331061   | 1.881757    | -3.336934   | 1.886016    | -3.334889   | 1.887801    |
| F15| -3.521077   | -0.665907   | -3.527530   | -0.665992   | -3.526430   | -0.662089   |
| H16| -1.172079   | -1.809250   | -1.174923   | -1.812027   | -1.177025   | -1.811135   |

| At | MP2_FC/VQZ | CCSD(T)_FC/VTZ | CCSD(T)_AE/CVQZ |
|----|------------|----------------|----------------|
|    | x          | y              | x              | y              | x              | y              |
| C1 | 0.000000   | 0.000000       | 0.000000       | 0.000000       | 0.000000       | 0.000000       |
| C2 | 0.000000   | 0.000000       | 0.000000       | 1.403456       | 0.000000       | 1.398300       |
| N3 | 1.328866   | 1.312866       | 1.317152       | 1.894424       | 1.313279       | 1.888547       |
| C4 | 2.245888   | 2.245888       | 2.252471       | 0.875116       | 2.245082       | 0.873485       |
| C5 | 1.405903   | 1.405903       | 1.410305       | -0.445478      | 1.405635       | -0.444249      |
| C6 | -1.191057  | -1.191057      | -1.191458      | 2.119002       | -1.186484      | 2.112198       |
| C7 | -2.384523  | -2.384523      | -2.388562      | 1.390982       | -2.379418      | 1.387131       |
| C8 | -2.362388  | -2.362388      | -2.369698      | -0.003310      | -2.359810      | -0.001831      |
| C9 | -1.178858  | -1.178858      | -1.184519      | -0.730136      | -1.180551      | -0.727793      |
| O10| 3.451001   | 3.451001       | 3.454476       | 0.980218       | 3.442513       | 0.977031       |
| O11| 1.872120   | 1.872120       | 1.874976       | -1.560462      | 1.869448       | -1.554026      |
| H12| 1.566407   | 1.566407       | 1.570864       | 2.867666       | 1.566763       | 2.860124       |
| H13| -1.210145  | -1.210145      | -1.207232      | 3.201205       | -1.201427      | 3.192495       |
| H14| -3.339616  | -3.339616      | -3.343883      | 1.898898       | -3.333316      | 1.893781       |
| F15| -3.531512  | -3.531512      | -3.542365      | -0.660416      | -3.530825      | -0.657132      |
| H16| -1.177136  | -1.177136      | -1.185224      | -1.812075      | -1.182320      | -1.807991      |
Table S4. Calculated harmonic and anharmonic wavenumbers (cm\(^{-1}\)) of 1-methylisatin in comparison with experimental vibrational spectra in the gas phase.

| No | Observed [1] | Calculated | Assignment (PED, %) |
|----|--------------|------------|---------------------|
|    | IR | Raman | harm | anharm | v, α, γ, τ |
| v₁ | – | – | 3223 | 3102 | ν₁₃₅(45), ν₁₅₅(23), ν₁₁₇(17), ν₉₁₆(15) |
| v₂ | – | – | 3217 | 3062 | ν₆₁₃(63), ν₈₁₅(20), ν₉₁₆(15) |
| v₃ | – | – | 3206 | 3051 | ν₆₁₆(65), ν₉₁₇(17) |
| v₄ | – | – | 3194 | 3016 | ν₇₁₄(66), ν₉₁₅(19) |
| v₅ | – | – | 3164 | 3002 | ν₁₂₁₇(86) |
| v₆ | 2948 w | 2950 m | 3109 | 2938 | ν₁₂₁₉(50), ν₁₂₁₆(50) |
| v₇ | – | – | 3049 | 2866 | ν₁₂₁₆(43), ν₁₂₁₆(43) |
| v₈ | 1743 s | 1740 vs | 1800 | 1781 | ν₁₄₁₀(66), ν₁₁₁(20) |
| v₉ | 1718 vs | 1717 s | 1789 | 1772 | ν₅₁₅(68), ν₄₁₀(19) |
| v₁₀ | 1603 vs | 1610 vs | 1660 | 1619 | ν₁₆₁₆(26), ν₁₆₁₆(16) |
| v₁₁ | – | – | 1641 | 1597 | ν₂₁₂(22), ν₂₁₆(16), ν₁₁₂(15) |
| v₁₂ | 1486 sh | – | 1533 | 1492 | α₁₁₂₁₉(43) |
| v₁₃ | 1467 vs | – | 1513 | 1470 | α₁₁₂₁₉(15) |
| v₁₄ | – | 1488 w | 1509 | 1450 | α₁₇₁₂₁₉(46), α₁₇₁₂₁₉(46) |
| v₁₅ | – | 1456 w | 1509 | 1450 | α₆₇₁₄(14), α₈₆₁₄(12), ν₆₁₆(12), ν₉₁₆(12) |
| v₁₆ | – | – | 1461 | 1420 | α₁₃₁₂₁₅(23), α₁₃₁₂₁₅(18), α₁₇₁₂₁₉(18) |
| v₁₇ | 1364 s | – | 1406 | 1359 | α₃₁₂(18) |
| v₁₈ | 1325 vs | 1328 s | 1371 | 1324 | ν₃₁₄(11), ν₃₁₂₁₁₁₈, ν₉₁₆(11) |
| v₁₉ | – | 1308 w | 1348 | 1311 | ν₂₁₂(12), α₆₆₁₃(12) |
| v₂₀ | 1253 m | 1253 vs | 1273 | 1237 | α₃₁₂₁₅(15), ν₃₁₄(15) |
| v₂₁ | 1192 m | 1194 m | 1214 | 1188 | ν₁₂₁₆(26) |
| v₂₂ | 1161 m | 1161 m | 1187 | 1165 | α₆₇₁₄(21), α₆₇₁₄(18) |
| v₂₃ | – | – | 1160 | 1122 | α₁₃₁₂₁₆(46), α₃₁₂₁₆(46) |
| v₂₄ | 1111 s | 1117 s | 1138 | 1111 | α₁₃₁₂₁₅(13), α₉₈₁₆(10) |
| v₂₅ | 1089 vs | 1091 sh | 1113 | 1085 | ν₈₁₆(11), ν₈₁₆(9) |
| v₂₆ | 1035 m | – | 1052 | 1022 | ν₁₂₁₆(42) |
| v₂₇ | – | 1019 s | 1042 | 1018 | ν₁₂₁₆(30), ν₈₁₆(16), ν₈₁₆(15) |
| v₂₈ | – | – | 987 | 969 | γ₁₄₁₁₆(30), γ₁₅₁₁₆(27) |
| v₂₉ | 993 sh | – | 968 | 948 | γ₁₆₁₆(43), γ₁₄₁₆(21) |
| v₃₀ | 955 m | 956 w | 962 | 941 | ν₄₁₄(17) |
| v₃₁ | 880 m | 865 w | 881 | 855 | γ₁₁₁₆(45) |
| v₃₂ | 863 s | 879 | 864 | α₃₄₁₀(10), α₉₈₁₆(9) |
| v₃₃ | 816 m | 817 w | 832 | 801 | γ₁₁₁₆(39), γ₁₀₁₄(30) |
| v₃₄ | 757 vs | – | 771 | 747 | γ₁₅₁₆(35), γ₁₄₁₆(17), γ₁₃₁₆(15) |
| v₃₅ | – | – | 732 | 711 | γ₆₁₆(30), γ₁₀₁₄(15) |
| v₃₆ | 701 s | 703 vs | 714 | 702 | α₂₆₁₇(13), α₉₈₁₆(11) |
| v₃₇ | 684 m | 685 m | 696 | 688 | α₂₆₁₇(11), α₁₅₁₁₆(10) |
| v₃₈ | 543 m | – | 561 | 541 | α₁₅₁₆(16) |
| v₃₉ | 556 m | 560 m– | 558 | 553 | γ₁₀₁₈(18), γ₁₀₁₈(16) |
| v₄₀ | – | 527 s | 533 | 523 | ν₁₂₁₆(22), |
| v₄₁ | – | 483 vs | 487 | 471 | ν₂₁₁(11), α₂₆₁₆(10) |
| v₄₂ | 473 vs | – | 485 | 479 | γ₁₀₁₈(31), γ₁₁₁₆(23), γ₁₀₁₄(15) |
| v₄₃ | – | – | 407 | 395 | γ₆₁₄(20), γ₁₀₁₄(16), γ₁₁₁₆(15) |
| v₄₄ | – | 328 m | 327 | 324 | α₅₄₁₀(24), α₅₄₁₀(20), ν₅₁₆(16) |
| v₄₅ | 296 m | – | 293 | 291 | α₂₃₁₂₁₅(15) |
| v₄₆ | – | 252 w | 273 | 260 | γ₁₂₁₆(26), γ₉₁₆(19) |
| v₄₇ | – | 161 m | 237 | 239 | α₂₃₁₂₁₅(17), α₅₁₆(16), α₁₀₁₆(15) |
| v₄₈ | – | – | 157 | 31 | γ₁₂₁₆(85) |
| v₄₉ | – | 171 m | 140 | 243 | γ₉₁₆(20), γ₁₁₁₆(18) |
| v₅₀ | – | – | 123 | 119 | γ₁₂₁₆(39), τ₁₂₁₆(27), τ₁₄₁₆(21) |
| v₅₁ | – | – | 102 | 95 | τ₄₁₆(29), τ₁₂₁₆(23), τ₁₂₁₆(20) |

\( \nu \); stretching. \( \alpha \); bending. \( \gamma \); wagging. \( \tau \); torsion.

\( \nu \); very. s; strong. w; weak. m; medium. sh; shoulder. PED; potential energy distribution.
Table S5. Total corrections $\Delta(r_{ij,e} - r_{ij,a})$ to internuclear distances $r_{ij,a}$, theoretical $u_{ij,ht}$ and experimental $u_{ij,exp}$ rms vibrational amplitudes (in Å) for 1-methyolisatin, Å.

| Parameter | $r_{ij,a}$ | $r_{ij,e} - r_{ij,a}^a$ | $u_{ij,ht}^b$ | $u_{ij,exp}$ |
|-----------|------------|--------------------------|---------------|--------------|
| C1--C2    | 1.409      | 0.0066                   | 0.0461        | 0.0486(21)$^c$ |
| C2--N3    | 1.411      | 0.0098                   | 0.0467        | 0.0492(21)$^c$ |
| N3--C4    | 1.390      | 0.0108                   | 0.0469        | 0.0494(21)$^c$ |
| C4--C5    | 1.568      | 0.0080                   | 0.0563        | 0.0588(21)$^c$ |
| C1--C5    | 1.481      | 0.0071                   | 0.0501        | 0.0526(21)$^c$ |
| C2--C6    | 1.392      | 0.0073                   | 0.0451        | 0.0476(21)$^c$ |
| C6--C7    | 1.407      | 0.0066                   | 0.0460        | 0.0485(21)$^c$ |
| C7--C8    | 1.402      | 0.0072                   | 0.0458        | 0.0483(21)$^c$ |
| C8--C9    | 1.402      | 0.0064                   | 0.0458        | 0.0483(21)$^c$ |
| C1--C9    | 1.391      | 0.0069                   | 0.0450        | 0.0475(21)$^c$ |
| C4--O10   | 1.209      | 0.0036                   | 0.0376        | 0.0401(21)$^c$ |
| C5--O11   | 1.208      | 0.0042                   | 0.0375        | 0.0400(21)$^c$ |
| N3--C12   | 1.455      | 0.0119                   | 0.0484        | 0.0509(21)$^c$ |
| C$^a$Ph--H| 1.103      | 0.0151                   | 0.0751        | 0.0751        |
| C12--H17  | 1.102      | 0.0162                   | 0.0759        | 0.0759        |
| C12--H18  | 1.106      | 0.0158                   | 0.0767        | 0.0767        |
| O10...O11 | 3.032      | 0.0130                   | 0.1030        | 0.1197(103)$^d$ |
| N3...O10  | 2.317      | 0.0088                   | 0.0543        | 0.0601(58)$^c$ |
| N3...O11  | 3.494      | 0.0110                   | 0.0596        | 0.0758$^d$    |
| C1...O11  | 2.422      | 0.0074                   | 0.0595        | 0.0653(58)$^e$ |
| C4...O11  | 2.469      | 0.0091                   | 0.0673        | 0.0731(58)$^e$ |
| C5...O10  | 2.513      | 0.0087                   | 0.0674        | 0.0732(58)$^e$ |
| O10...C12 | 2.905      | 0.0029                   | 0.1039        | 0.1206(103)$^d$ |
| C9...O11  | 3.202      | 0.0045                   | 0.0975        | 0.1142(103)$^d$ |
| C2...O10  | 3.470      | 0.0057                   | 0.0572        | 0.0734(112)$^f$ |
| C2...O11  | 3.479      | 0.0066                   | 0.0572        | 0.0734(112)$^f$ |
| C1...O10  | 3.612      | 0.0055                   | 0.0604        | 0.0766(112)$^f$ |
| C8...O11  | 4.566      | 0.0041                   | 0.0956        | 0.1932(242)$^g$ |
| C6...O10  | 4.755      | 0.0061                   | 0.0678        | 0.1654(242)$^g$ |
| C6...O11  | 4.763      | 0.0045                   | 0.0652        | 0.1628(242)$^g$ |
| O11...C12 | 4.851      | 0.0018                   | 0.0756        | 0.1732(242)$^g$ |
| C9...O10  | 4.971      | 0.0031                   | 0.0701        | 0.1677(242)$^g$ |
| C7...O11  | 5.172      | 0.0032                   | 0.0842        | 0.1818(242)$^g$ |
| C7...O10  | 5.843      | 0.0034                   | 0.0678        | 0.1519(569)$^h$ |
| C8...O10  | 5.962      | 0.0028                   | 0.0683        | 0.1524(569)$^h$ |
| C1...N3   | 2.331      | 0.0128                   | 0.0532        | 0.0590(58)$^e$ |
| N3...C5   | 2.340      | 0.0143                   | 0.0564        | 0.0622(58)$^e$ |
| N3...C6   | 2.506      | 0.0138                   | 0.0607        | 0.0665(58)$^f$ |
| N3...C9   | 3.625      | 0.0151                   | 0.0589        | 0.0751(112)$^f$ |
| N3...C7   | 3.736      | 0.0156                   | 0.0637        | 0.0799(112)$^f$ |
| N3...C8   | 4.197      | 0.0167                   | 0.0653        | 0.1629(242)$^g$ |
| C2...C4   | 2.312      | 0.0087                   | 0.0542        | 0.0600(58)$^e$ |
| C2...C5   | 2.307      | 0.0098                   | 0.0547        | 0.0605(58)$^e$ |

(to be continued)
| Parameter | \( r_{ij,a} \) | \( r_{ij,c} - r_{ij,a} \) | \( u_{ij,h1} \) | \( u_{ij,exp} \) |
|-----------|---------------|----------------|--------------|--------------|
| C2..C7    | 2.392         | -0.0100        | 0.0556       | 0.0614(58)   |
| C1..C8    | 2.429         | -0.0092        | 0.0556       | 0.0614(58)   |
| C1..C4    | 2.437         | -0.0082        | 0.0568       | 0.0626(58)   |
| C7..C9    | 2.403         | -0.0083        | 0.0560       | 0.0618(58)   |
| C2..C9    | 2.415         | -0.0100        | 0.0561       | 0.0619(58)   |
| C1..C6    | 2.441         | -0.0078        | 0.0565       | 0.0623(58)   |
| C6..C8    | 2.459         | -0.0097        | 0.0562       | 0.0620(58)   |
| C4..C12   | 2.496         | -0.0049        | 0.0692       | 0.0750(58)   |
| C2..C12   | 2.528         | -0.0129        | 0.0704       | 0.0762(58)   |
| C5..C9    | 2.645         | -0.0063        | 0.0663       | 0.0721(58)   |
| C1..C7    | 2.777         | -0.0084        | 0.0637       | 0.0804(103)  |
| C2..C8    | 2.801         | -0.0117        | 0.0631       | 0.0798(103)  |
| C6..C9    | 2.814         | -0.0088        | 0.0631       | 0.0798(103)  |
| C6..C12   | 3.068         | -0.0210        | 0.1070       | 0.1237(103)  |
| C4..C6    | 3.650         | -0.0113        | 0.0624       | 0.0786(112)  |
| C5..C6    | 3.639         | -0.0106        | 0.0602       | 0.0764(112)  |
| C1..C12   | 3.709         | -0.0096        | 0.0669       | 0.0831(112)  |
| C5..C12   | 3.744         | -0.0081        | 0.0685       | 0.0847(112)  |
| C4..C9    | 3.814         | -0.0083        | 0.0644       | 0.0806(112)  |
| C5..C8    | 3.869         | -0.0088        | 0.0682       | 0.0844(112)  |
| C5..C7    | 4.221         | -0.0096        | 0.0689       | 0.1665(242)  |
| C7..C12   | 4.458         | -0.0188        | 0.1075       | 0.2051(242)  |
| C4..C7    | 4.670         | -0.0105        | 0.0650       | 0.1626(242)  |
| C4..C8    | 4.765         | -0.0100        | 0.0656       | 0.1632(242)  |
| C9..C12   | 4.912         | -0.0110        | 0.0766       | 0.1742(242)  |
| C8..C12   | 5.239         | -0.0153        | 0.0962       | 0.1938(242)  |

\( ^a \) Calculated with the B2PLYP/cc-pVTZ cubic force constants (see text).

\( ^b \) Calculated with the B2PLYP/cc-pVTZ quadratic force constants (see text).

\( ^c,d,e,f,g,h \) Amplitudes with the same superscript were refined in one group. Differences between amplitudes in each group were fixed at the corresponding calculated values. Other amplitudes were assumed at the calculated values. 3\( \sigma \) Values for groups \( ^c,d,e,f,g,h \) are 0.002, 0.010, 0.006, 0.011, 0.024 and 0.057, respectively.

Reference

[1] T. Polat, F. Bulut, I. Arıcan, F. Kandemirli, and G. Yıldırım, J. Mol. Struct. **1101**, 189 (2015).