

Supporting Information

for

Tandem processes promoted by a hydrogen shift in 6-arylfulvenes bearing acetalic units at *ortho* position: a combined experimental and computational study

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Computational details

All calculations were carried out with the Gaussian09¹ suite of programs. An intensive characterization of the potential energy surface was done at the HF/6-31G*² theoretical level and then with the hybrid three-parameter functional customarily denoted as B3LYP³ using the 6-31+G** basis set. All the reported stationary points were fully optimized by analytical gradient techniques. Harmonic frequency calculations at each level of theory verified the identity of each stationary point as a minimum or a transition state, and were used to provide an estimation of the zero-point vibrational energies (ZPVE), which were not scaled. The intrinsic reaction coordinates (IRC)⁴ were followed to verify the energy profiles connecting each transition state to the correct local minima, by using the second-order Gonzalez–Schlegel integration method.⁵

To evaluate the influence of the DMSO solvent ($\epsilon = 47$), we have optimized all the stationary points at the B3LYP/6-31+G** calculations using a Self-Consistency Reaction Field (SCRF)⁶ method, based on the Polarized Continuum Model (PCM)⁷ of Tomasi and co-workers.

¹ Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

² Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. in *Ab Initio Molecular Orbital Theory*, Wiley, New York, **1986**, pp 71-82, and references cited therein.

³ (a) Parr, R. G.; Yang, W. *Density-Functional Theory of Atoms and Molecules*, Oxford University Press, New York, 1989. (b) Bartolotti, L. J.; Fluchichk, K. in *Reviews in Computational Chemistry*, Lipkowitz, K. B.; Boyd, D. B. Eds. VCH Publishers, New York, **1996**, Vol. 7; pp 187-216. (c) Kohn, W.; Becke, A. D.; Parr, R. G. *J. Phys. Chem.* **1996**, *100*, 12974–12980. (d) Ziegler, T. *Chem. Rev.* **1991**, *91*, 651–667.

⁴ (a) Fukui, K. *J. Phys. Chem.* **1970**, *74*, 4161-4162. (b) Fukui, K. *Acc. Chem. Res.* **1981**, *14*, 363-368.

⁵ (a) Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523-5527. (b) Gonzalez, C.; Schlegel, H. B. *J. Chem. Phys.* **1991**, *95*, 5853-5860.

⁶ (a) Tomasi, J.; Persico, M. *Chem. Rev.* **1994**, *94*, 2027–2094; (b) Simkin, B. Y.; Sheikhet, I. *Quantum Chemical and Statistical Theory of Solutions: A Computational Approach*; Ellis Horwood: London, UK, **1995**, pp 78–101.

⁷ (a) Miertus, S.; Scrocco, E.; Tomasi, J. *J. Chem. Phys.* **1981**, *55*, 117–129; (b) Cammi, R.; Tomasi, J. *J. Chem. Phys.* **1994**, *100*, 7495–7502; (c) Barone, V.; Cossi, M.; Tomasi, J. *J. Chem. Phys.* **1997**, *107*, 3210–3221.

Table S1. Electronic energies (hartrees) of the stationary points found in the conversions **3a** → **5a** + **6a** and **5a** → **27a** → **6a** calculated at the B3LYP/6-31+G** and PCM-B3LYP/6-31+G** (using dimethylsulfoxide as solvent) theoretical levels. The ZPVE corrections calculated at each level of calculation have been included and are not scaled.

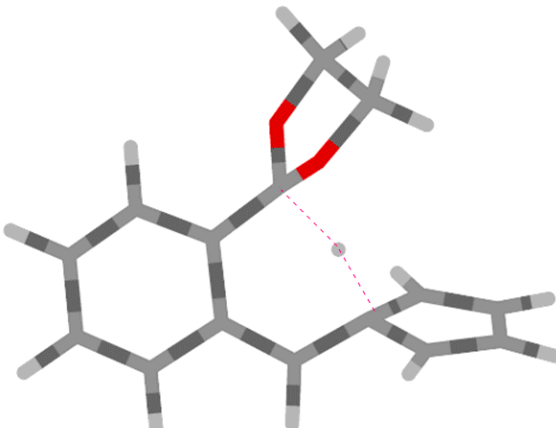
3a → 5a + 6a 5a → 27a → 6a	B3LYP/6-31+G**	PCM-B3LYP/6-31+G**
3a	-730,19741	-730,18543
TS1-A	-730,12172	-730,10998
9a	-730,15407	-730,14395
TS2	-730,12292	-730,11360
10a	-730,16904	-730,15961
TS3	-730,12385	-730,11585
10a'	-730.16757	-730,15848
TS4	-730,15646	-730,14747
TS5	-730,12358	-730,11604
11a	-730,16464	-730,15593
TS1-B	-730,13145	-730,12184
TS1-C	-730,09494	-730,08414
TS6	-730,14252	-730,13296
13a	-730,22680	-730,21490
TS7	-730,14187	-730,13172
12a	-730,21712	-730,20582
TS8	-730,16042	-730,15631
5a	-730,24734	-730,23610
TS9	-730,15217	-730,14640
6a	-730,24639	-730,23467
TS10	-730,17849	-730,16872
TS11	-730,17843	-730,16925
27a	-730,19966	-730,18837

Table S2. Relative electronic (E) and Gibbs (G) energies in kcal·mol⁻¹ of the stationary points found in the conversions **3a** → **5a** + **6a** and **5a** → **27a** → **6a** calculated at B3LYP/6-31+G** and PCM-B3LYP/6-31+G** (using dimethylsulfoxide as solvent) theoretical levels. The ZPVE corrections calculated at each level of calculation have been included and are not scaled.

3a → 5a + 6a 5a → 27a → 6a	E	G	$E_{(\text{DMSO})}$	$G_{(\text{DMSO})}$
3a	0.0	0.0	0.0	0.0
TS1-A	47.5	49.5	47.3	49.3
9a	27.2	27.9	26.0	26.9
TS2	46.7	47.5	45.1	46.2
10a	17.8	18.8	16.2	17.7
TS3	46.2	47.5	43.7	45.1
10a'	18.7	19.4	16.9	18.3
TS4	25.7	27.4	23.8	25.6
TS5	46.3	47.2	43.5	44.8
11a	20.6	21.5	18.5	18.9
TS1-B	41.4	43.5	39.9	42.2
TS1-C	64.3	66.4	63.6	65.9
TS6	34.4	36.0	32.9	34.8
13a	-18.4	-16.0	-18.5	-15.8
TS7	34.8	36.3	33.7	35.7
12a	-12.4	-10.0	-12.8	-10.7
TS8	23.2	25.8	18.3	20.9
5a	-31.3	-30.9	-31.8	-30.8
TS9	28.4	31.0	24.5	26.9
6a	-30.7	-30.2	-30.9	-29.8
TS10	11.9	12.3	10.5	11.9
TS11	11.9	12.4	10.2	11.3
27a	-1.4	-1.3	-1.8	-0.9

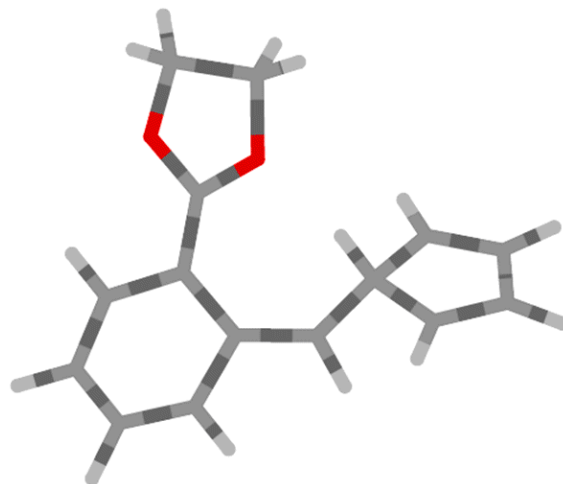
Cartesian coordinates and geometries of the stationary points found in the transformations **3a** $\rightarrow$ **5a** + **6a** and **5a** $\rightarrow$ **27a** $\rightarrow$ **6a** optimized at the B3LYP/6-31+G** theoretical level.

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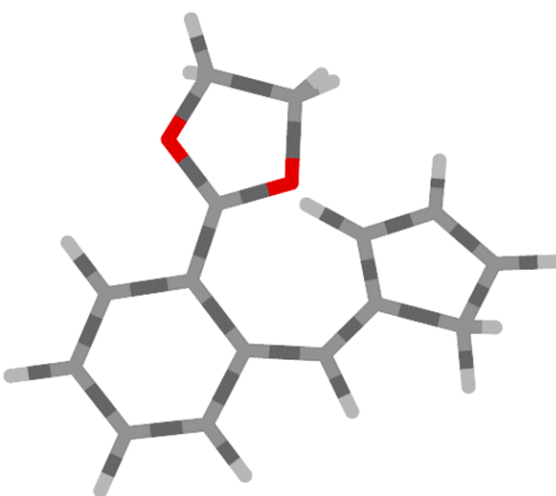
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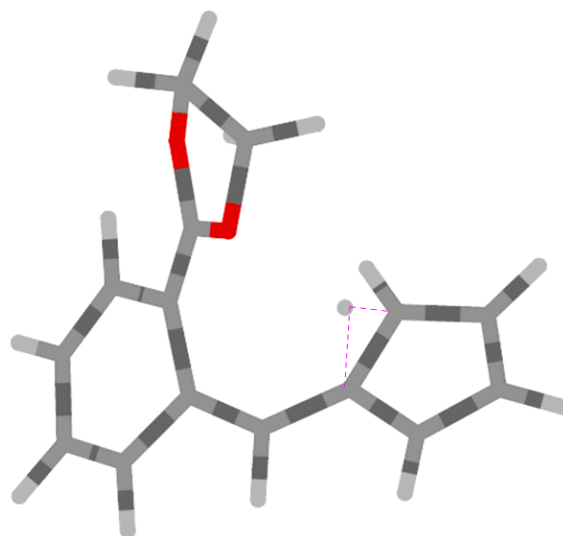
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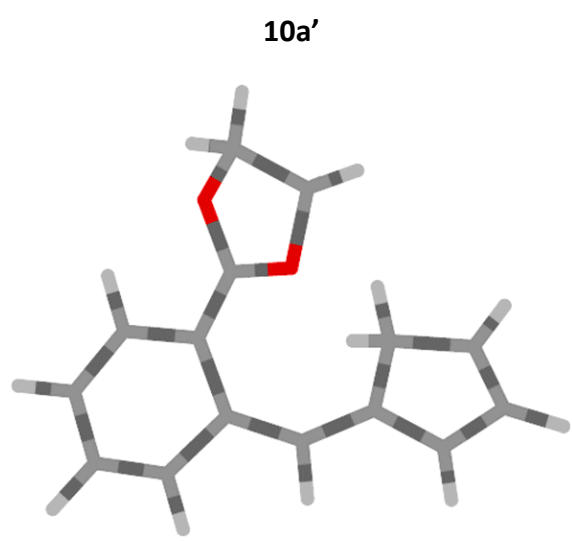
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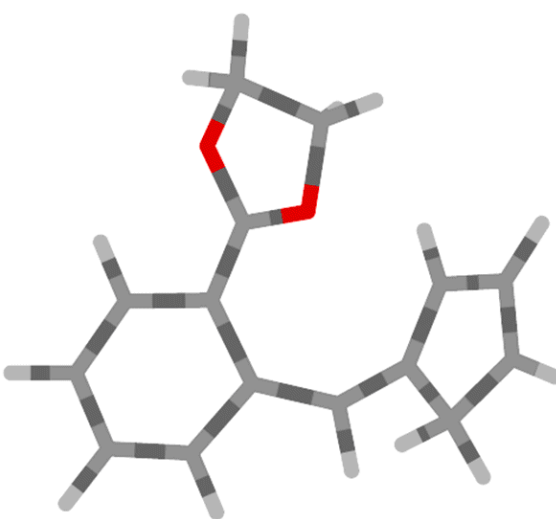
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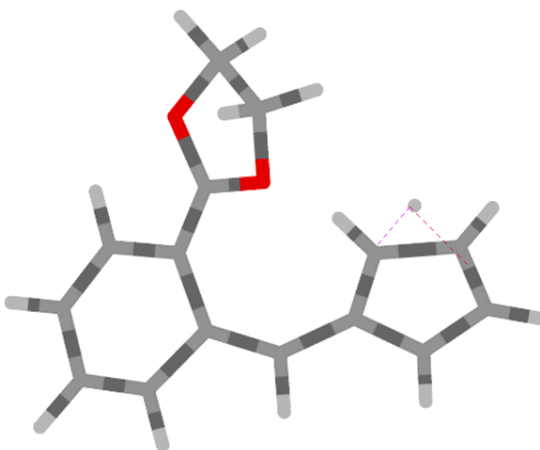
TS3

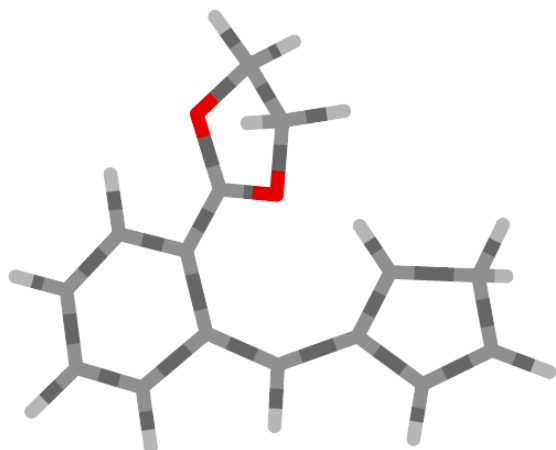


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 Sum of electronic and thermal energies=
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 Sum of electronic and thermal enthalpies=
 -730.109169
 Sum of electronic and thermal Free energies=
 -730.164763

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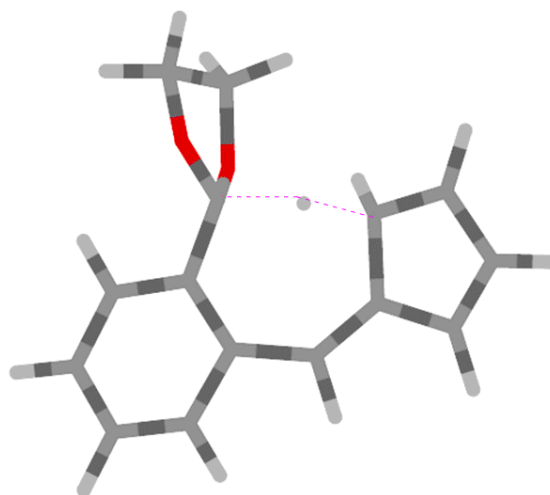
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	Freq: -41.2599 Sum of electronic and zero-point energies= -730.156455 Sum of electronic and thermal energies= -730.143037 Sum of electronic and thermal enthalpies= -730.142093 Sum of electronic and thermal Free energies= -730.196915

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	Freq: -1261.6447 Sum of electronic and zero-point energies= -730.123580 Sum of electronic and thermal energies= -730.109626 Sum of electronic and thermal enthalpies= -730.108682 Sum of electronic and thermal Free energies= -730.165325

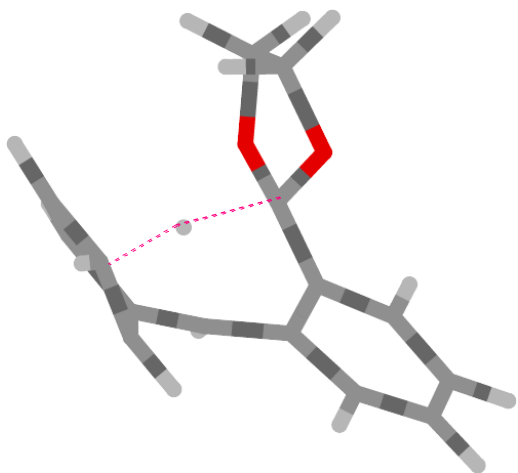
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	Freq: 47.1729 Sum of electronic and zero-point energies= -730.164637 Sum of electronic and thermal energies= -730.150450 Sum of electronic and thermal enthalpies= -730.149505 Sum of electronic and thermal Free energies= -730.206328

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 C,-0.7941736041,0.6583888738,1.1349951643
 C,0.173051553,0.7491560142,0.0699327932
 C,1.2911264551,-0.1145008962,-0.1599881705
 C,1.7027518637,-1.2790791597,0.475654071
 C,1.3876056578,-1.7316456562,1.8807071421
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 C,2.2149663899,-3.5028199148,0.6626281747
 C,2.2728312807,-2.3936850871,-0.1937812685
 C,-0.1569387303,1.6157983387,-1.0211910028
 C,-1.3797666643,2.238214621,-1.1330266818
 C,-2.3713544816,2.0092518243,-0.1526554919
 C,-2.0836924931,1.2201105135,0.9430358693
 H,0.1886010065,-1.2610567618,2.0534244361
 H,1.7454194467,0.0361063543,-1.139050422
 H,1.7993346481,-1.1032196984,2.6748409136
 H,1.6693639658,-3.7505846216,2.7994487611
 H,2.532293857,-4.5062531738,0.3967507118
 H,2.5369972105,-2.4146585649,-1.2447803996
 H,0.5780000699,1.7329625669,-1.812975256
 H,-1.5906673259,2.8754799948,-1.9866513155
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 H,-2.8255704635,1.0695742927,1.7185914477
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 H,0.6428255999,0.9046725962,5.2116686683
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 H,-1.7641614552,1.0357638975,4.7762272053

TS1-B

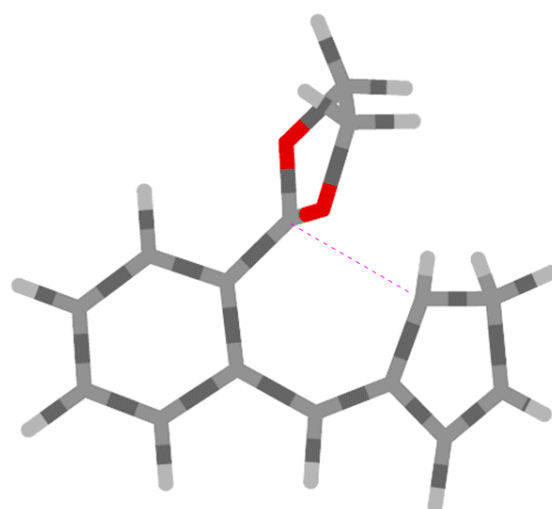


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 Sum of electronic and thermal enthalpies=
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 Sum of electronic and thermal Free energies=
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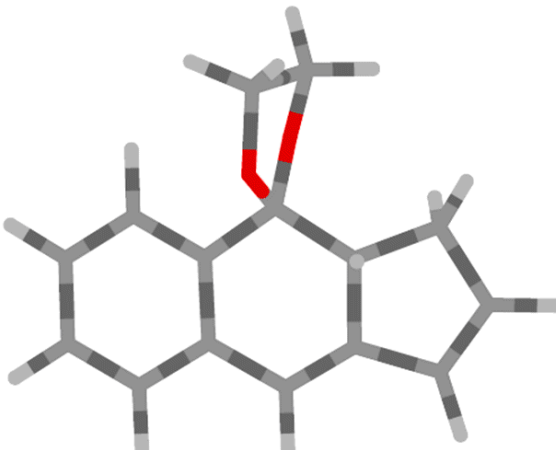
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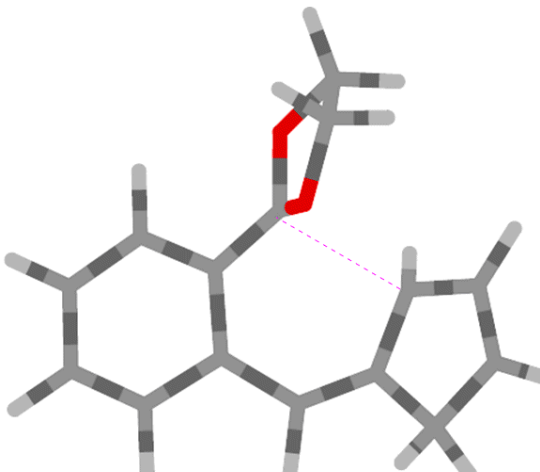
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 C,1.0035433045,-1.4079250736,0.9920203391
 C,2.0237903549,-0.6087435224,0.4503366891
 C,3.3562205362,-1.1592827241,0.1328788079
 C,4.0400653967,-0.3054647108,-0.6547873571
 C,3.2279875505,0.9452708685,-0.8873239627
 C,1.9532515518,0.6898246467,-0.1014039599
 C,-1.0971520172,-2.6333544277,0.7677363161
 C,-2.1792502586,-2.9591205017,-0.0146396086
 C,-2.5841553028,-2.0997072202,-1.070265562
 C,-1.952470812,-0.8881897004,-1.2445290328
 H,3.7452308781,1.8504244887,-0.5353655911
 H,1.3246112539,-2.3043177749,1.520378268
 H,3.6783833042,-2.1524485512,0.430255944
 H,4.9989531336,-0.4986367994,-1.1234882955
 H,3.0477251859,1.100710516,-1.9632106541
 H,1.5172700636,1.5005189822,0.4541650116
 H,-0.7387630626,-3.3333244381,1.5182110712
 H,-2.705673804,-3.8948501688,0.1519774204
 H,-3.4212740406,-2.3724380651,-1.7057548621
 H,-2.30030761,-0.1918617779,-1.9996167458
 O,-0.5045405846,1.6096641105,0.7955192342
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 C,-0.6114033713,3.0419601179,-1.0430683639
 C,-0.740737586,2.99558491,0.4828546597
 H,0.3941779116,3.3316600448,-1.369568726
 H,-1.3563947206,3.6698763681,-1.534215491
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 H,-1.7452532031,3.2586148028,0.8310430536

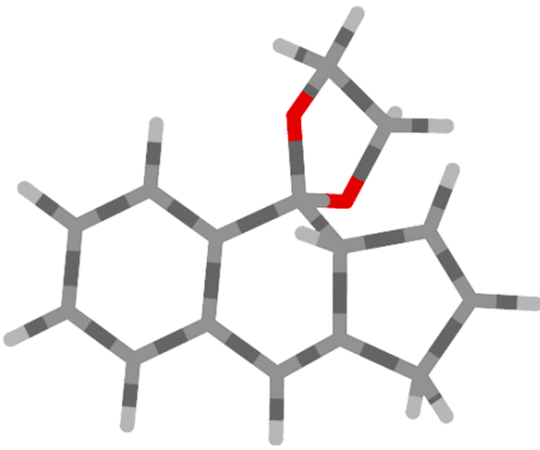
TS6

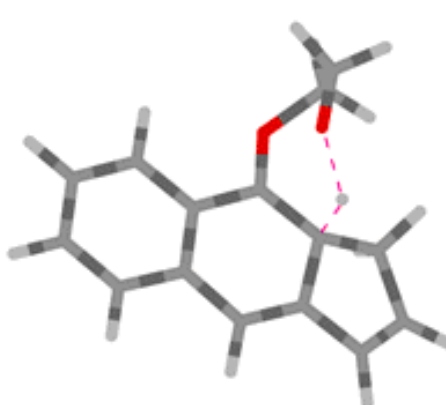


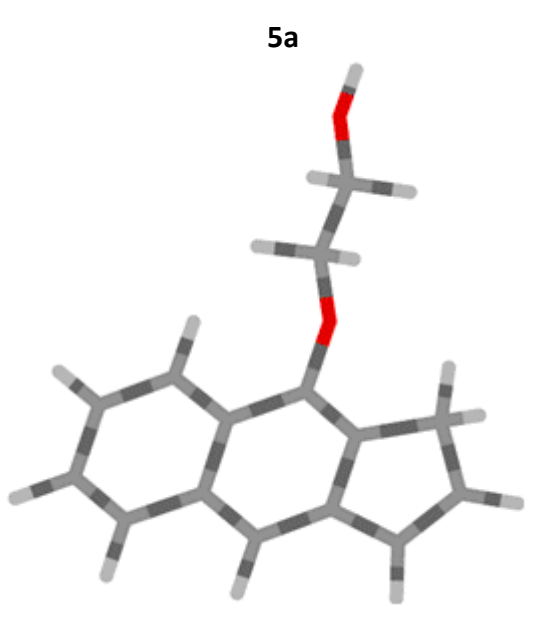
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 Sum of electronic and thermal enthalpies=
 -730.128225
 Sum of electronic and thermal Free energies=
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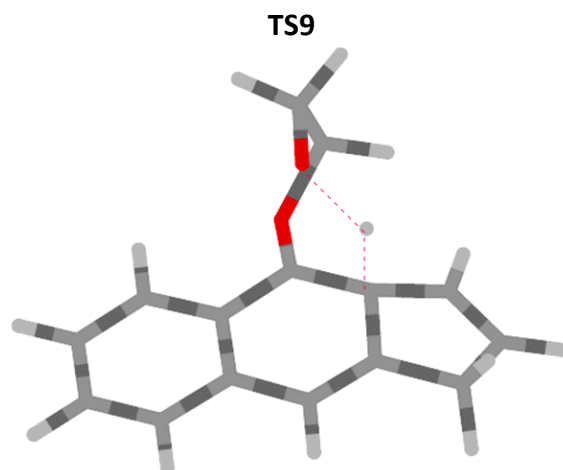
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C,-0.4192124352,0.6568843835,0.356876695 C,1.0290461822,0.152855231,0.3599314235 C,1.2788741092,-1.1715737946,-0.0792255723 C,0.1526921386,-2.0591522028,-0.3975104766 C,-1.0874480676,-1.7478844746,0.005217042 C,-1.3541982278,-0.4732989254,0.7921451239 C,-2.8445183029,-0.2851233346,0.6213581134 C,-3.4146347298,-1.3563489416,0.0565853838 C,-2.406585882,-2.4333854645,-0.2946038127 C,2.6081112836,-1.6052508422,-0.1968567263 C,3.6713583665,-0.7638177197,0.1368590579 C,3.4169259639,0.5284786655,0.5996284087 C,2.0962998664,0.980694603,0.706134299 H,-2.557356595,-3.3349035005,0.3203744635 H,0.355919751,-2.9624058483,-0.9692610541 H,-1.1149921715,-0.6345500443,1.8582612138 H,-3.3712752665,0.5940639578,0.9766792929 H,-4.4794099817,-1.4743745491,-0.1203212545 H,-2.4758243836,-2.7578739316,-1.3411495345 H,2.8050193468,-2.6170369649,-0.5427490898 H,4.693324666,-1.1208515795,0.0458419696 H,4.2379068354,1.1819275329,0.8801746813 H,1.8910199031,1.9774396844,1.0820669628 O,-0.7870889966,1.0990391335,-0.9537044347 O,-0.564290507,1.7976797157,1.2118952553 C,-0.9438643596,2.9315175484,0.4224967824 C,-0.569960269,2.5067435704,-0.9963478413 H,-2.0219549937,3.1136586495,0.5209572391 H,-0.3947056364,3.8073908985,0.7815821532 H,-1.2147241257,2.9250046924,-1.7726869449 H,0.479511519,2.7362768515,-1.2286708194	12a 
	Freq: 58.6197 Sum of electronic and zero-point energies= -730.217122 Sum of electronic and thermal energies= -730.204253 Sum of electronic and thermal enthalpies= -730.203309 Sum of electronic and thermal Free energies= -730.256437

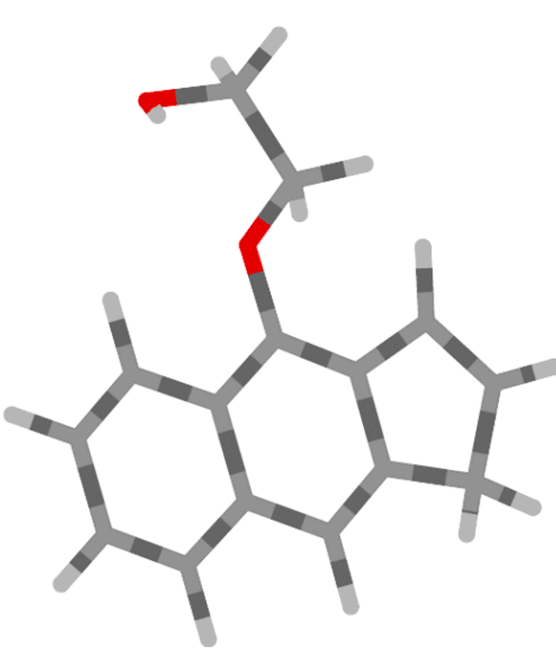
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	Freq: -1033.8935 Sum of electronic and zero-point energies= -730.160420 Sum of electronic and thermal energies= -730.147438 Sum of electronic and thermal enthalpies= -730.146494 Sum of electronic and thermal Free energies= -730.199341

C,0.22797,0.132669,-0.351356 C,-0.788108,-0.866113,-0.193639 C,-2.119046,-0.453843,0.162922 C,-2.411829,0.928233,0.335043 C,-1.412268,1.858842,0.151194 C,-1.426695,3.322239,0.230596 C,-0.20051,3.81032,-0.049564 C,0.778601,2.694699,-0.344881 C,-0.08047,1.459696,-0.192179 C,-3.116474,-1.455399,0.324515 C,-2.825897,-2.790243,0.138147 C,-1.517102,-3.189257,-0.226686 C,-0.522197,-2.246782,-0.389719 H,1.20622,2.772931,-1.354228 H,-3.422078,1.229918,0.59937 H,-2.305479,3.909324,0.474749 H,0.075214,4.858812,-0.067712 H,1.631072,2.708779,0.348457 H,5.495236,-1.386792,0.51294 H,-4.12269,-1.146373,0.596226 H,-3.602496,-3.538973,0.265386 H,-1.298202,-4.241609,-0.382872 H,0.47732,-2.546441,-0.685467 O,4.643527,-1.088268,0.853758 O,1.503808,-0.259346,-0.721025 C,2.412934,-0.471258,0.368621 C,3.737616,-0.9108,-0.234749 H,2.551395,0.453435,0.942956 H,2.028253,-1.243901,1.046381 H,4.094092,-0.140972,-0.932983 H,3.594308,-1.845243,-0.794658	5a  Freq: 29.0683 Sum of electronic and zero-point energies= -730.247338 Sum of electronic and thermal energies= -730.232850 Sum of electronic and thermal enthalpies= -730.231906 Sum of electronic and thermal Free energies= -730.289776
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C,-0.0197419769,0.3335836826,-0.3201158159
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 C,1.3308052337,-1.5128604993,0.6330733604
 C,0.1524163567,-2.3490977044,0.7095888296
 C,-1.0477890629,-1.8734279026,0.3100270089
 C,-1.2078490122,-0.5385319028,-0.3095004433
 C,-2.620329167,-0.1464480197,0.0376771153
 C,-3.3049571978,-1.21310438,0.4783673372
 C,-2.4286601363,-2.4482951294,0.5514567543
 C,2.5846896644,-1.981318902,1.0789329126
 C,3.703362758,-1.1605298801,1.0692923204
 C,3.6099756588,0.1680620763,0.6137714956
 C,2.3938764174,0.6553569319,0.1646883679
 H,-2.4954589267,-2.975120436,1.5108346631
 H,0.2451959407,-3.3280720108,1.1729503792
 H,-1.1011367765,-0.6309076227,-1.5166240386
 H,-3.0376524661,0.8411362063,-0.1168777484
 H,-4.362946269,-1.2212897106,0.7170269164
 H,-2.709397939,-3.1761329882,-0.2268864973
 H,2.6632751688,-3.0036071265,1.4386638511
 H,4.657494101,-1.5467179108,1.416766836
 H,4.4892008509,0.8046631908,0.6052097727
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 O,-0.0919608529,-0.0871036446,-2.5388685694
 O,-0.0913840679,1.6411670304,-0.581936908
 C,-0.8467571282,2.0358353252,-1.762415994
 C,-0.2752203403,1.2143237013,-2.9394563795
 H,-1.9091061894,1.8317470824,-1.6058877
 H,-0.6940361011,3.1136090988,-1.8514411737
 H,-0.9890449077,1.3262729209,-3.7785070578
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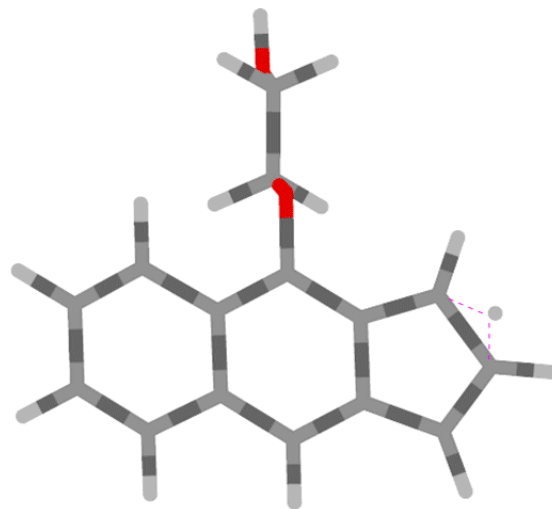


Freq: -1159.3763
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 Sum of electronic and thermal energies=
 -730.139110
 Sum of electronic and thermal enthalpies=
 -730.138166
 Sum of electronic and thermal Free energies=
 -730.191098

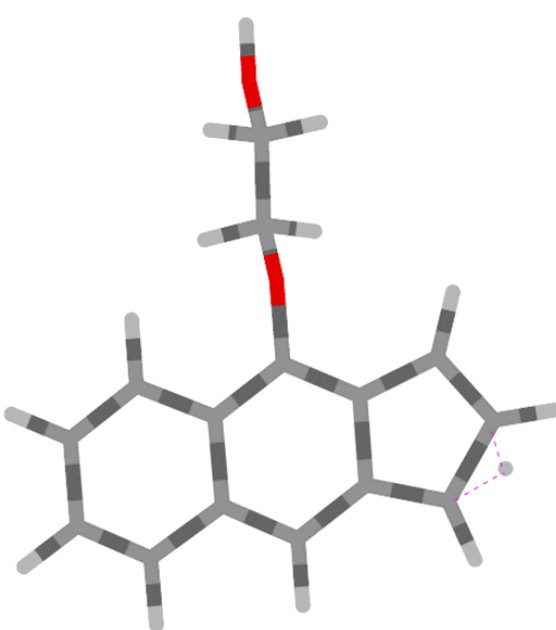
C,-0.3822507412,0.4182821483,0.0105846201 C,0.9129016356,-0.0858469285,0.3406836351 C,1.0148964363,-1.2720476935,1.1470270991 C,-0.1695845638,-1.9189902542,1.6108811378 C,-1.395719188,-1.3962940903,1.2914097671 C,-1.5115041727,-0.2158253915,0.4887752292 C,-2.9342408476,0.0989633444,0.3448520783 C,-3.6724928559,-0.8206406989,1.0015885716 C,-2.7913379686,-1.858526242,1.6611450154 C,2.3092290909,-1.7647839706,1.4650992018 C,3.4464628697,-1.122963466,1.0202109789 C,3.3401106304,0.0514413801,0.2353787055 C,2.1016560144,0.5607469022,-0.0969636421 H,-2.9428501941,-1.8894088589,2.7493100487 H,-0.0770070315,-2.8151617503,2.2201184502 H,1.4519196019,2.2390845278,-3.476143059 H,-3.3194198976,0.9555517298,-0.1956360265 H,-4.7545430554,-0.8312145309,1.0700159062 H,-3.0035012148,-2.8716958454,1.2911985216 H,2.3891550611,-2.6616921441,2.0743910048 H,4.4269554046,-1.5138607693,1.2767604971 H,4.2409963169,0.5577693761,-0.0995233758 H,2.0114808769,1.4699531797,-0.6822018535 O,1.0100702732,2.9170381388,-2.9480989265 O,-0.469163961,1.5696273492,-0.7497733078 C,-0.7345320846,1.3676185771,-2.1429201027 C,-0.385634452,2.6368449884,-2.9029736571 H,-0.1424161943,0.5190300815,-2.5167254219 H,-1.7979882133,1.1290033591,-2.2961843857 H,-0.8085990638,2.5642490286,-3.9168119526 H,-0.8442175115,3.4959025232,-2.4053507573	6a  Freq: 28.0509 Sum of electronic and zero-point energies= -730.246393 Sum of electronic and thermal energies= -730.232093 Sum of electronic and thermal enthalpies= -730.231149 Sum of electronic and thermal Free energies= -730.288664
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C,0.237020808,0.1029678943,-0.3360339284
 C,-0.7783984916,-0.8521940226,-0.1936787435
 C,-2.1271021447,-0.4155475031,0.1468859282
 C,-2.4159638201,0.9382921117,0.3280090253
 C,-1.3961295324,1.900033855,0.1885279833
 C,-1.4140890222,3.308265069,0.2781289062
 C,-0.1108797517,3.7857490711,-0.0268824517
 C,0.7738041619,2.6132145088,-0.263847947
 C,-0.0478445135,1.4694605291,-0.1542880856
 C,-3.1414186399,-1.4241738438,0.2871272337
 C,-2.8621354925,-2.7506579585,0.1023801351
 C,-1.5388332778,-3.1714122146,-0.2437391563
 C,-0.5339763464,-2.2527531954,-0.3864410199
 H,0.1382716911,3.5140344627,-1.1988687986
 H,-3.4286157692,1.2425991348,0.579192601
 H,-2.2739530224,3.9300923154,0.4873294163
 H,0.2629966501,4.7874938901,0.1554169703
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 H,5.529149883,-1.3114631602,0.5579613307
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 H,-3.6470437875,-3.4933449441,0.2136082467
 H,-1.3370956244,-4.2274286997,-0.3982434125
 H,0.4664160291,-2.5654468708,-0.6650208974
 O,4.6788720759,-1.0013817854,0.8920070889
 O,1.5137654605,-0.2888768977,-0.6906892191
 C,2.431031925,-0.4535634966,0.4023868017
 C,3.7631170964,-0.8778059896,-0.1956265731
 H,2.5475844981,0.4871868086,0.9547403194
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 H,4.0977378735,-0.1203491923,-0.9181143449
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TS10

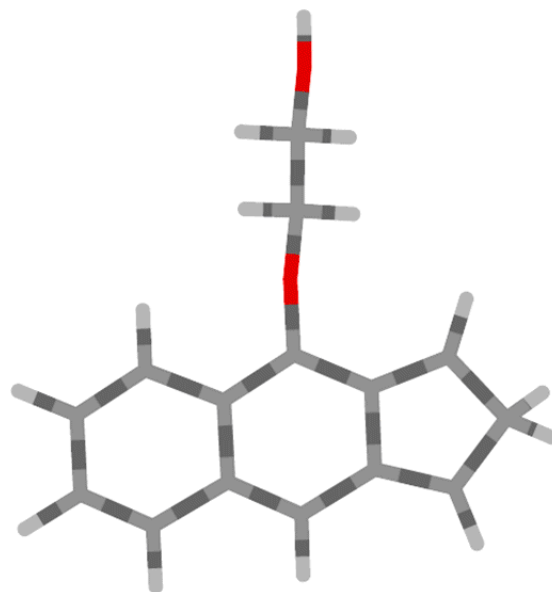


Freq: -1170.3313
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 Sum of electronic and thermal energies=
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 Sum of electronic and thermal enthalpies=
 -730.163231
 Sum of electronic and thermal Free energies=
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	Freq: -1174.9072 Sum of electronic and zero-point energies= -730.178430 Sum of electronic and thermal energies= -730.164117 Sum of electronic and thermal enthalpies= -730.163173 Sum of electronic and thermal Free energies= -730.220808

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 C,-2.402296563,0.915312812,0.3591994384
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 C,-1.363647653,3.2505134069,0.2986395495
 C,0.0125161984,3.7554847606,-0.0087192425
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 C,0.0026119041,1.4336156755,-0.1662922613
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 C,-1.5858856564,-3.193373793,-0.2500088373
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 H,0.0103410838,4.4480378258,-0.8662228909
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 H,1.8634619238,2.5307589742,-0.5780681533
 H,5.6236944878,-1.1363513603,0.4102403565
 H,-4.1651831123,-1.0907271422,0.5698445509
 H,-3.7028344453,-3.4819795101,0.2233322016
 H,-1.4071491148,-4.2531282838,-0.4070826395
 H,0.4247824655,-2.6291040533,-0.6824442769
 O,4.769179393,-0.8707531956,0.7707724587
 O,1.5080129854,-0.3969847458,-0.7032921277
 C,2.4828611765,-0.437274382,0.3528356517
 C,3.8070596146,-0.8299193123,-0.2826384613
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 H,2.1881465648,-1.1779534303,1.107171412
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27a



Freq: 27.5925
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 Sum of electronic and thermal energies=
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 Sum of electronic and thermal enthalpies=
 -730.183954
 Sum of electronic and thermal Free energies=
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