

Supplementary Material

A new divalent organoeuropium(II) fluoride and serendipitous discovery of an alkoxide complex from pentaphenylcyclopentadiene precursors

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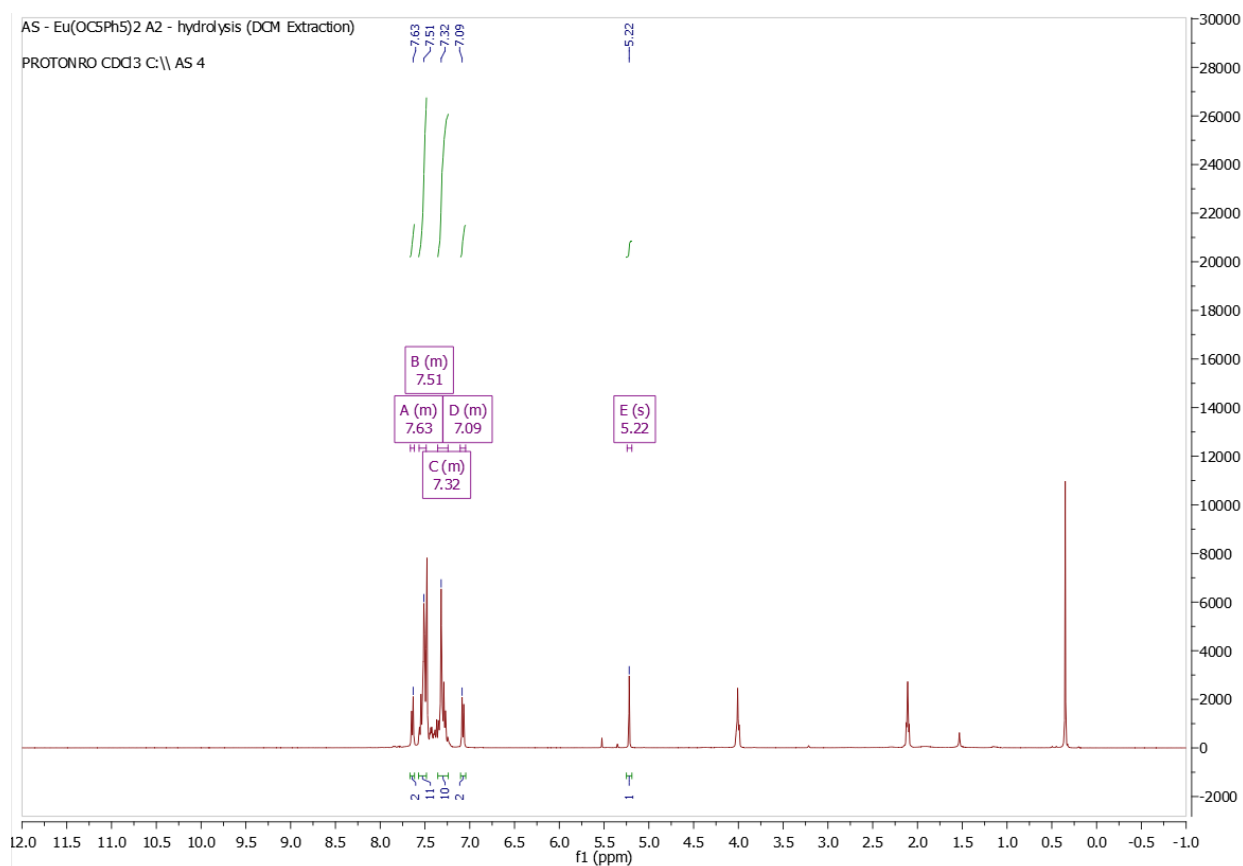


Figure S1. ^1H NMR spectrum of **3**

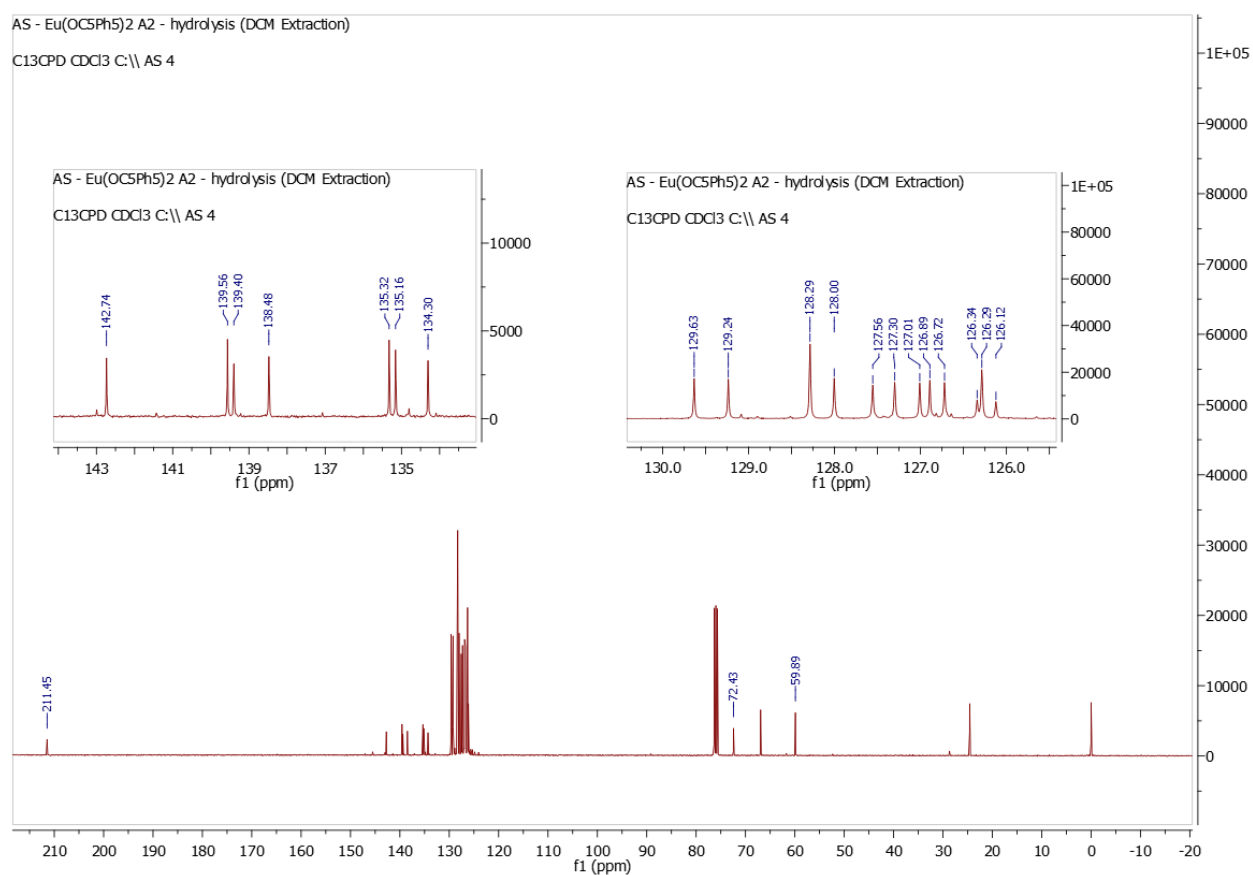


Figure S2. ^{13}C NMR spectrum of **3** with expansions

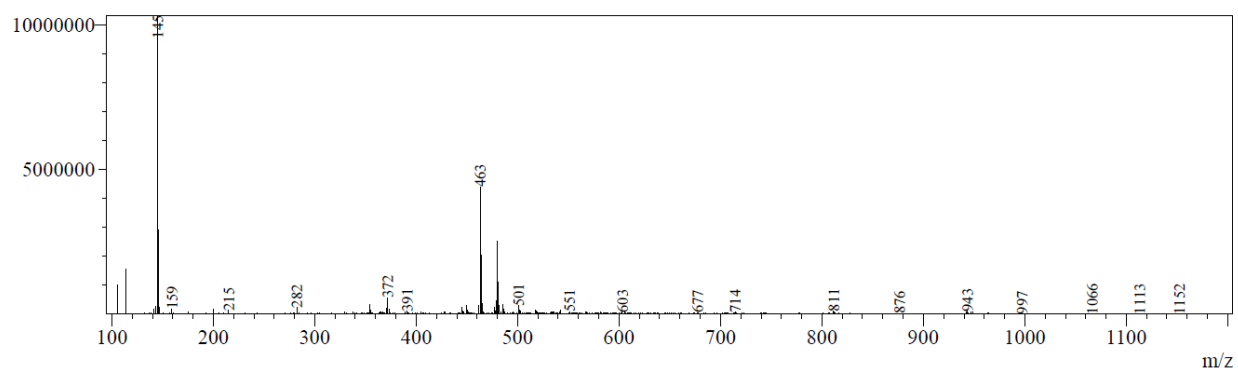


Figure S3. Mass spectrum of **3** showing molecular ion at 463 m/z .

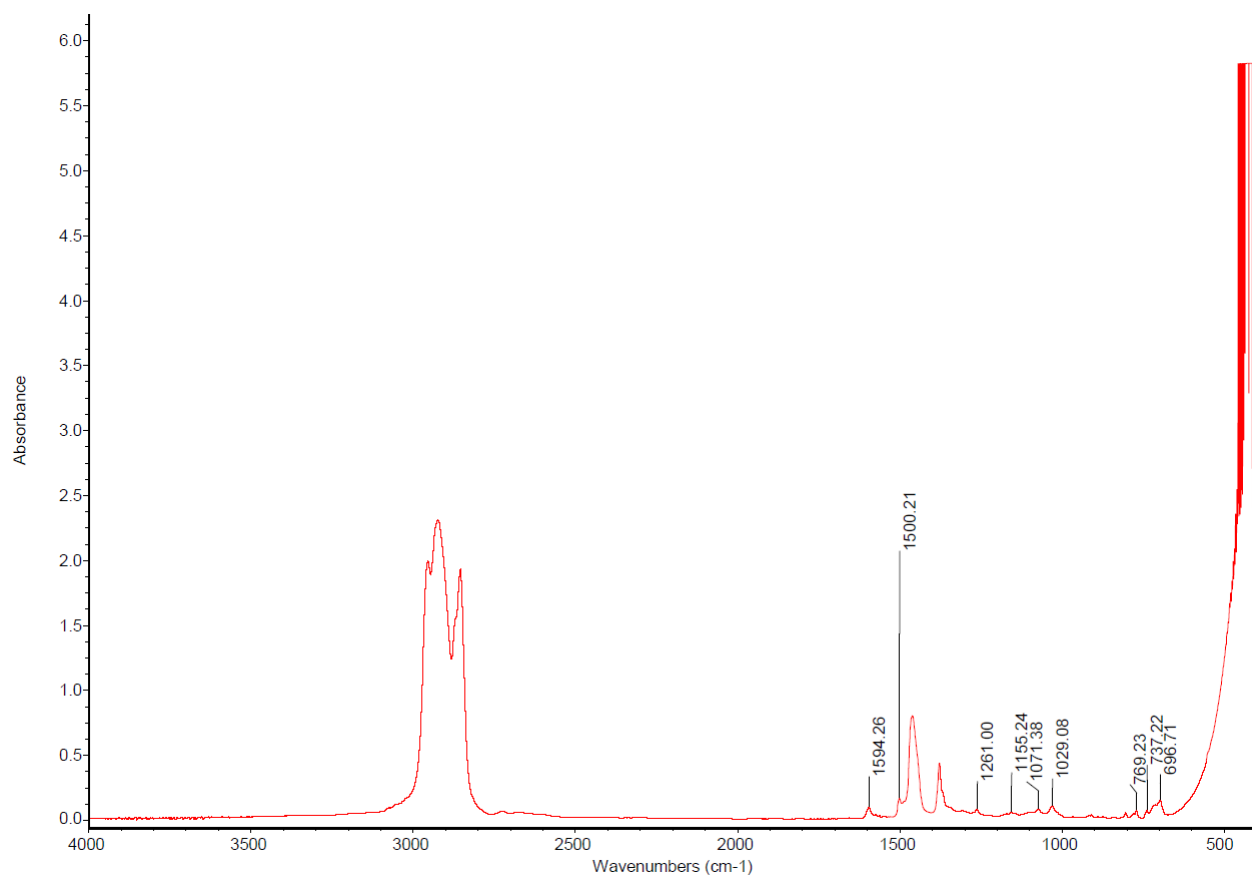


Figure S4. Infrared spectrum of **1** (Nujol mull)

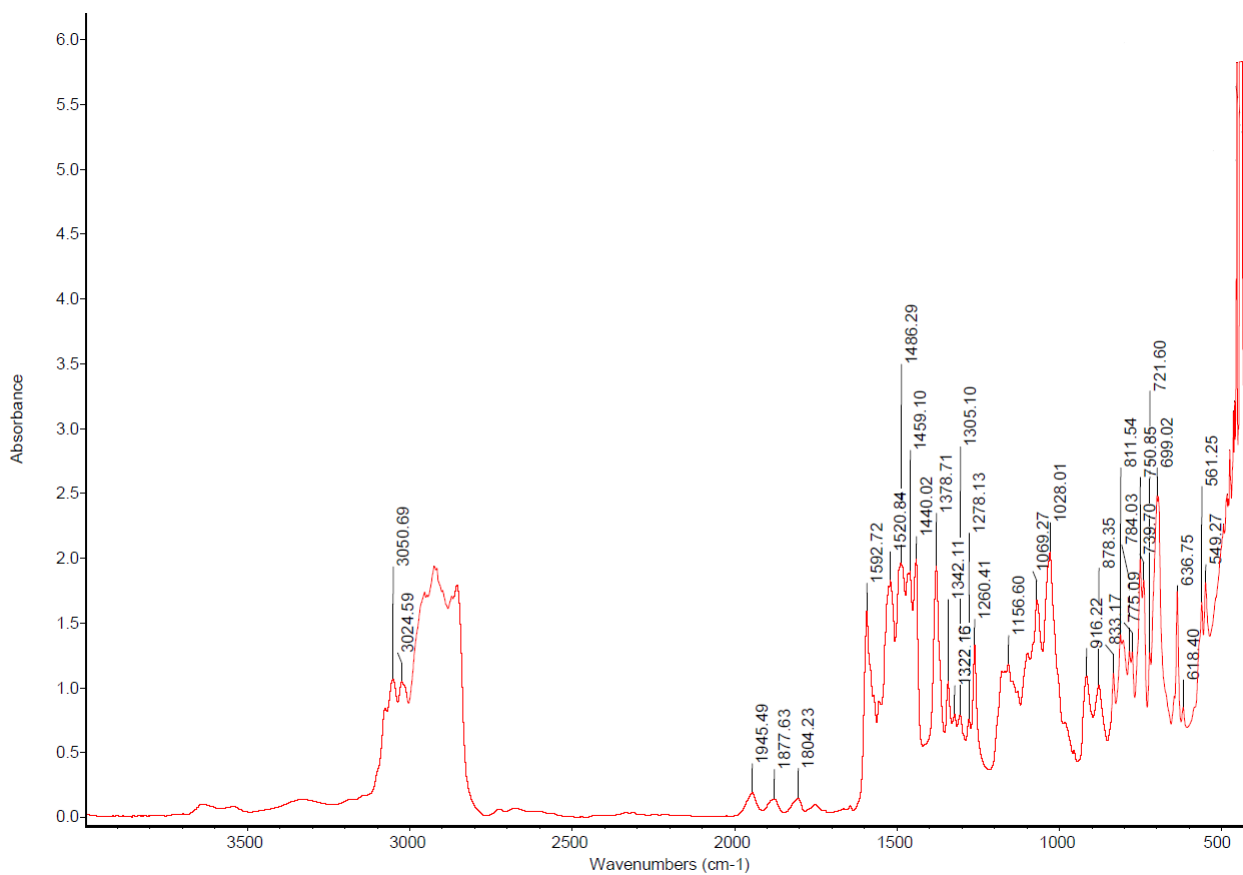


Figure S5. Infrared spectrum of **2** (Nujol mull)

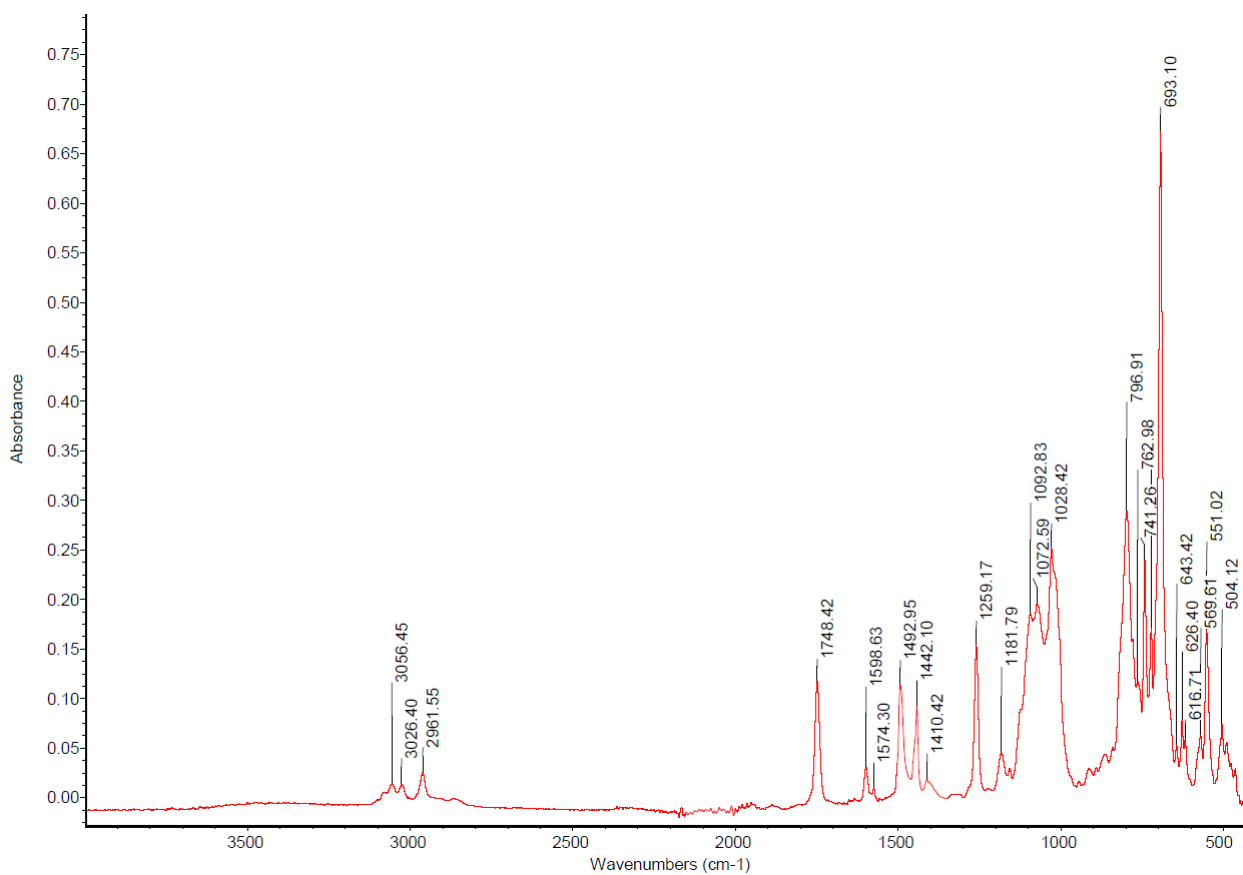


Figure S6. Infrared spectrum of **3** (ATR)

X-ray crystallography:

Single crystals of **1** were covered with viscous hydrocarbon oil and were mounted on loops. Data were obtained at 123 K on a Bruker X8 APEX II CCD diffractometer equipped with graphite-monochromated Mo- $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$). For complex **2**, a single crystal covered with oil based cryoprotectant was mounted on a cryoloop. The single crystal X-ray diffraction measurement was carried out at 100 K on a Bruker D8 Venture equipped with a fine-focus sealed tube with a Triumph graphite monochromator displaying Mo $K_{\alpha 1}$ wavelength ($\lambda = 0.7103 \text{ \AA}$) and a PHOTON100 CMOS detector. Data were collected using Bruker Apex2 software. Single crystals of C_5Ph_5OH were coated with viscous hydrocarbon oil and mounted on glass loops, and data were collected on a Rigaku SynergyS diffractometer. The SynergyS operated using microsource Cu- $K\alpha$ radiation ($\lambda = 1.54178 \text{ \AA}$) at 123 K. Data processing was conducted using CrysAlisPro.55 software suite.^[1] Single crystals of **3** were mounted on loops. Data were obtained at 190 K on an Oxford Diffraction Gemini Ultra S diffractometer, using Cu- $K\alpha$ radiation ($\lambda = 1.54184 \text{ \AA}$). The structures were solved using SHELXS7 and refined by full-matrix least-squares on all F2 data using SHELX2014^[2] in conjunction with the X-Seed graphical user interface.^[3] All hydrogen atoms were placed in calculated positions using the riding model.

Table S1. Crystal data and structural refinement for compounds **1**, **2**, **3** and C₅Ph₅OH·H₂O

	1	2	3	-
	[Eu(C ₅ Ph ₅)(μ-F)(thf) ₂] ₂	[Eu(OC ₅ Ph ₅ [*]) ₂ (thf) ₄]	C ₅ P ₅ H=O	C ₅ Ph ₅ OH·H ₂ O
Empirical formula	C ₈₆ H ₈₂ Eu ₂ F ₂ O ₄	C ₈₆ H ₈₂ O ₆ Eu	C ₃₅ H ₂₆ O	C ₃₅ H ₂₈ O ₂
Formula weight	1521.43	1363.47	462.56	480.57
Space group	Pbca	P2 ₁ /c	Pbca	P-1
a/Å	17.9079(7)	22.2767(11)	17.2715(4)	10.1622(3)
b/Å	19.1478(9)	11.1369(6)	17.1822(4)	10.2074(3)
c/Å	19.9962(9)	28.0596(15)	34.1838(8)	14.2703(2)
α/°	90	90	90	100.982(2)
β/°	90	104.3170(10)	90	90.324(2)
γ/°	90	90	90	116.247(2)
Volume/Å ³	6856.6(5)	6745.2(6)	10144.5(4)	1296.51(6)
Z	8	4	16	2
ρ _{calc} /cm ³	1.474	1.343	1.211	1.231
μ/mm ⁻¹	1.871	0.986	0.547	0.582
Reflections collected	87134	143124	30615	26972
Independent reflections	10120 [R _{int} = 0.0789, R _{sigma} = 0.0538]	20713 [R _{int} = 0.0613, R _{sigma} = 0.0507]	7841 [R _{int} = 0.0627, R _{sigma} = 0.0474]	5299 [R _{int} = 0.0521, R _{sigma} = 0.0362]
Goodness-of-fit on F ²	1.048	1.087	1.035	1.075
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0378, wR ₂ = 0.0749	R ₁ = 0.0462, wR ₂ = 0.0742	R ₁ = 0.0475, wR ₂ = 0.1015	R ₁ = 0.0416, wR ₂ = 0.1149
Final R indexes [all data]	R ₁ = 0.0727, wR ₂ = 0.0863	R ₁ = 0.0714, wR ₂ = 0.0805	R ₁ = 0.0738, wR ₂ = 0.1145	R ₁ = 0.0447, wR ₂ = 0.1179

Quantum chemical calculations were performed using CAM-B3LYP functional and Def2TZVP and Def2SVP basis sets included in Gaussian 09 software package^[4] for the gas phase. Stationary points on the potential energy surfaces were identified by calculating the corresponding Hessian matrices. The charges on atoms were calculated by the Mulliken method.

Table S2. Total and relative energies of the structures of the ground states **A-D**, **3** and the transition states **TS1-TS3** of the migrations of the phenyl group and the hydrogen atom for the gas phase calculated by the CAM-B3LYP/Def2TZVP method ^a

Structure	E_{total} , a.u.	E_{ZPE} , a.u.	ΔE_{ZPE} , kcal/mol	ω_1 , cm^{-1}
A	-1424.28983	-1423.78290	0	20
TS1	-1424.23167	-1423.72705	35.0	-658
B	-1424.28734	-1423.77992	1.9	17
TS3	-1424.17461	-1423.67358	68.6	-2308
3	-1424.29733	-1423.78998	-4.4	16
C	-1423.71651	-1423.22512	0	18
TS2	-1423.69260	-1423.20285	14.0	-382
D	-1423.75522	-1423.26259	-23.5	19

^a E_{total} is total energy (1 au = 627.5095 kcal/mol); E_{ZPE} is total energy corrected for zero point energy; ΔE_{ZPE} is the relative energy corrected for zero point energy; ω_1 , cm^{-1} is the lowest harmonic vibration frequency or the value of the single imaginary harmonic vibration frequency.

Table S3. Total and relative energies of the structures of the ground states **B**×MeOH and **3**×MeOH and the transition state **TS4** of the migrations of the hydrogen atom as well as energies of formation of complexes **B**×MeOH and **3**×MeOH for the gas phase calculated by the CAM-B3LYP/Def2SVP method ^{a,b}

Structure	E_{total} , a.u.	E_{ZPE} , a.u.	ΔE_{ZPE} , kcal/mol	E_f	$E_{f,ZPE}$	ω_1 , cm^{-1}
B ×MeOH	-1538.35676	-1537.79413	0	12.9	11.7	15
TS4	-1538.30632	-1537.74856	28.6			-1185
3 ×MeOH	-1538.36347	-1537.80064	-4.1	11.1	9.5	20

^a See designations in the Table S2 ^b E_f - energy of formation of a complex; $E_{f,ZPE}$ - energy of formation of a complex corrected for zero point energy (energy of formation of a complex was evaluated as the difference between the energy of a complex and the sum of the energies of individual molecules).

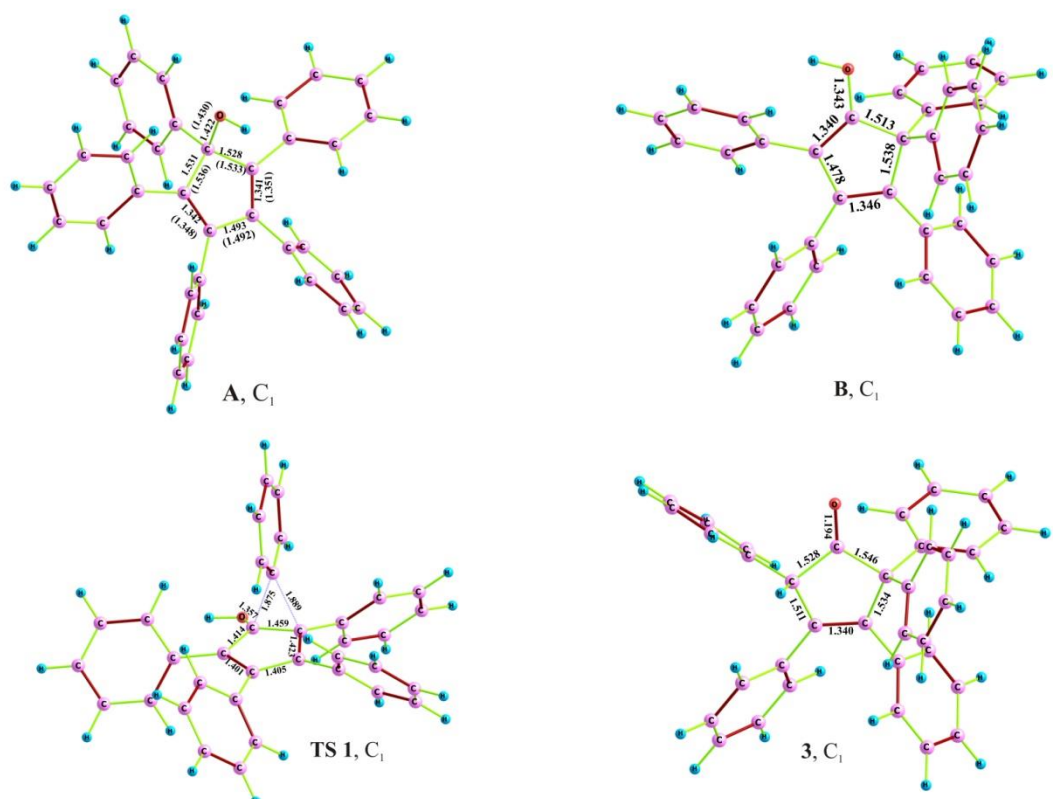


Figure S7. Calculated by CAM-B3LYP/Def2TZVP method geometric parameters of the structures of the ground state of **A**, **B** and **3** and transition state **TS1** corresponding to 1,5-sigmatropic shift of the phenyl group $\mathbf{A} \rightleftharpoons \mathbf{B}$ for the gas phase. For structure **A**, the bond lengths according to the data of X-ray structural analysis are given in parentheses. Hereinafter bond lengths are given in Å.

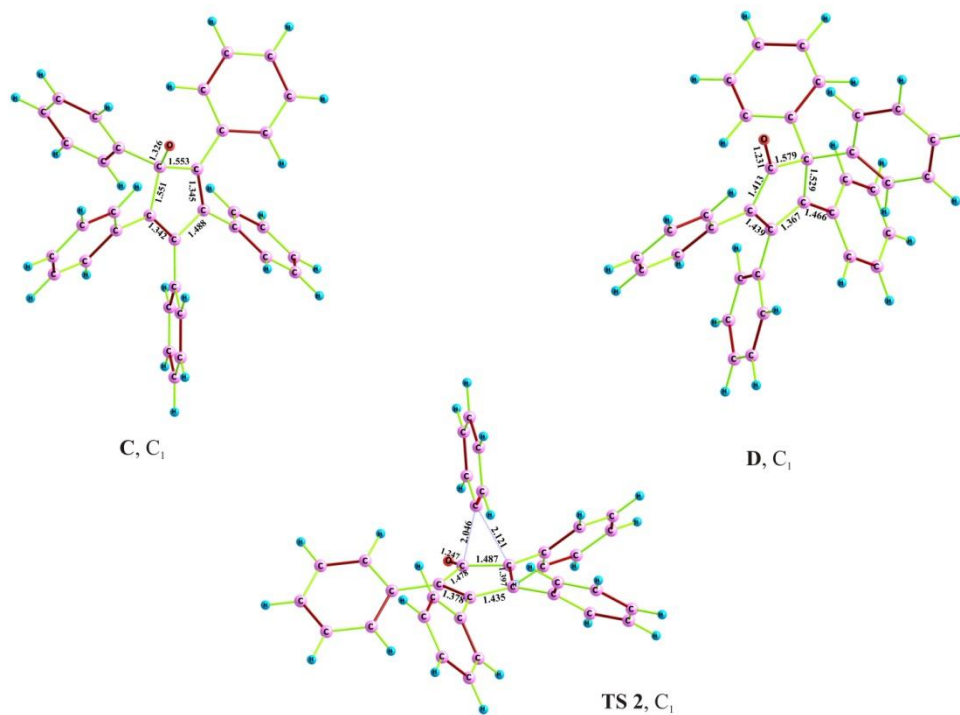


Figure S8. Calculated by CAM-B3LYP/Def2TZVP method geometric parameters of the structures of the ground state of the anions **C**, **D** and transition state **TS2** corresponding to 1,5-sigmatropic shift of the phenyl group **C**→**D** for the gas phase.

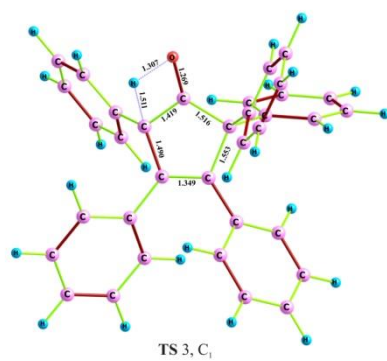


Figure S9. Calculated by CAM-B3LYP/Def2TZVP method geometric parameters of the structure of transition state **TS3** corresponding to 1,3-sigmatropic shift of the hydrogen atom **B**→**3** for the gas phase.

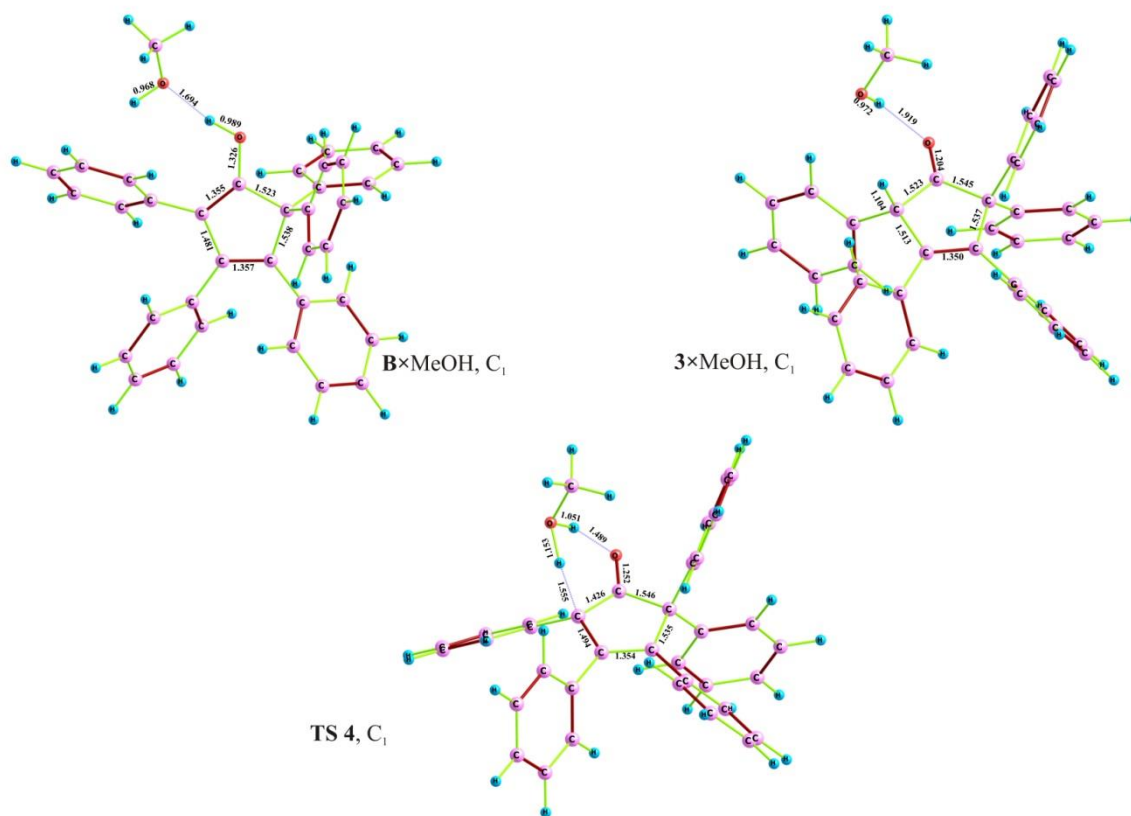


Figure S10. Calculated by CAM-B3LYP/Def2SVP method geometric parameters of the structures of the ground state of the complexes $B \times \text{MeOH}$ and $3 \times \text{MeOH}$ and transition state **TS4** corresponding to the migrations of the hydrogen atom for the gas phase.

Coordinates from computations at CAM-B3LYP/Def2TZVP level.

Structure A

6	-0.169743000	-1.296569000	-0.599414000
6	1.147323000	-0.563557000	-0.348931000
6	0.892761000	0.731015000	-0.108647000
6	-0.578146000	0.973870000	-0.191338000
6	-1.206516000	-0.175699000	-0.481017000
1	0.198432000	-1.262737000	-2.512062000
8	-0.159216000	-1.901052000	-1.886621000
6	2.456480000	-1.212857000	-0.542808000
6	3.397993000	-0.635236000	-1.394173000
6	2.784913000	-2.415275000	0.080896000
6	4.627182000	-1.231187000	-1.608892000
6	4.016919000	-3.008927000	-0.131164000
6	4.943014000	-2.421409000	-0.975840000
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1	2.076742000	-2.886964000	0.745697000
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1	4.252959000	-3.939170000	0.369006000
1	5.904310000	-2.889588000	-1.142010000
6	1.888718000	1.785212000	0.167849000
6	2.834554000	1.617585000	1.174816000
6	1.909808000	2.962874000	-0.574446000
6	3.780253000	2.595312000	1.427624000
6	2.860259000	3.937250000	-0.327771000
6	3.798317000	3.757708000	0.675251000
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1	1.177320000	3.116520000	-1.355634000
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1	-1.153768000	-5.117139000	3.074529000

Structure B

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6	-1.523073000	3.977513000	1.307990000
6	-2.765575000	3.492153000	-0.673486000
6	-2.476884000	4.347713000	0.374899000
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6	2.922643000	1.553219000	1.035432000
6	2.820341000	3.623010000	-0.792848000
6	3.856427000	2.572462000	1.091652000
6	3.809259000	3.611094000	0.176532000
1	1.108307000	2.622713000	-1.599177000
1	2.969210000	0.742348000	1.750612000
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1	4.626080000	2.553656000	1.852193000
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6	5.169213000	-2.727941000	-0.347968000
1	3.329122000	-0.231492000	-1.692627000
1	2.308994000	-2.958655000	1.434994000

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1	6.145428000	-3.186585000	-0.432167000
8	-0.004421000	-2.985690000	-0.272765000
1	0.860321000	-3.411724000	-0.335674000

Structure TS1

6	-1.068245000	-0.554767000	-0.456069000
6	0.060273000	-1.465839000	-0.611149000
6	1.261176000	-0.724612000	-0.530370000
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6	-0.734686000	-1.598518000	1.082050000
6	-0.227556000	-0.967117000	2.208070000
6	-0.441940000	-1.510032000	3.457648000
6	-1.176414000	-2.681328000	3.600698000
6	-1.688782000	-3.300482000	2.477299000
6	-1.470941000	-2.763056000	1.216344000
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6	-3.545903000	-0.494682000	-0.110465000
6	-2.681620000	-1.395651000	-2.154531000
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6	-3.974318000	-1.608700000	-2.605016000
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6	1.769986000	2.885480000	-0.864343000
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1	5.576084000	-0.911804000	-2.207297000
1	4.275826000	-4.124039000	0.291978000
1	6.029726000	-3.077779000	-1.103062000
8	-0.066131000	-2.669637000	-1.223561000
1	0.798658000	-3.100262000	-1.238620000

Structure C

6	-1.186174000	-0.239782000	-0.489469000
6	-0.155813000	-1.390972000	-0.630729000
6	1.167736000	-0.604313000	-0.429378000
6	-0.565345000	0.915579000	-0.205568000
6	0.903259000	0.682909000	-0.142038000
6	-0.395785000	-2.285648000	0.644743000
6	-0.260854000	-1.848906000	1.957903000
6	-0.509178000	-2.701982000	3.020269000
6	-0.904979000	-4.011041000	2.786816000
6	-1.048896000	-4.451310000	1.481449000
6	-0.796005000	-3.592790000	0.422214000
1	-0.394418000	-2.344523000	4.037160000
1	-1.362216000	-5.470891000	1.287005000
1	-1.100139000	-4.679221000	3.617041000
1	0.044268000	-0.827736000	2.152676000
1	-0.882668000	-3.891819000	-0.615657000
6	-2.622648000	-0.495768000	-0.636659000
6	-3.563077000	0.015380000	0.256966000
6	-3.070927000	-1.301633000	-1.686009000
6	-4.912430000	-0.247730000	0.097882000
6	-4.421609000	-1.561136000	-1.841292000
6	-5.349298000	-1.033068000	-0.956643000
1	-3.228426000	0.619444000	1.089490000
1	-2.314821000	-1.725165000	-2.336003000
1	-5.625255000	0.158053000	0.805542000
1	-4.753496000	-2.187116000	-2.661150000
1	-6.405352000	-1.239810000	-1.082034000
6	-1.198681000	2.235649000	-0.010683000
6	-0.969547000	2.987329000	1.140598000
6	-2.049579000	2.768492000	-0.977299000
6	-1.578082000	4.216406000	1.325992000
6	-2.658481000	3.997574000	-0.795039000
6	-2.427327000	4.728755000	0.358965000
1	-0.305802000	2.598957000	1.901842000
1	-2.234311000	2.199366000	-1.878483000
1	-1.386581000	4.777439000	2.232373000
1	-3.318013000	4.386609000	-1.560919000
1	-2.903125000	5.690714000	0.502472000
6	1.868576000	1.762523000	0.155249000
6	1.912118000	2.925868000	-0.609978000
6	2.755853000	1.649879000	1.223185000
6	2.821120000	3.931295000	-0.330023000
6	3.663569000	2.654758000	1.507984000
6	3.702358000	3.801237000	0.730875000
1	1.226938000	3.036923000	-1.439901000
1	2.733338000	0.751193000	1.825639000
1	2.839553000	4.822977000	-0.944307000
1	4.345459000	2.540647000	2.341568000
1	4.412340000	4.588271000	0.951763000
6	2.463137000	-1.241055000	-0.684444000
6	3.557227000	-0.528362000	-1.183195000
6	2.623350000	-2.617031000	-0.506127000
6	4.764280000	-1.149378000	-1.447108000

6	3.832487000	-3.237725000	-0.764180000
6	4.914176000	-2.509476000	-1.230013000
1	3.456792000	0.527253000	-1.386551000
1	1.784380000	-3.204371000	-0.170625000
1	5.590367000	-0.565989000	-1.835637000
1	3.923926000	-4.306027000	-0.610096000
1	5.858290000	-2.998103000	-1.437686000
8	-0.228528000	-2.075529000	-1.764603000

Structure D

6	-1.112183000	-0.739240000	0.026304000
6	0.096723000	-1.748056000	0.146716000
6	1.293312000	-0.996703000	0.137352000
6	-0.406185000	0.616608000	0.001554000
6	0.941961000	0.396933000	0.059228000
6	-1.995494000	-0.979958000	1.243626000
6	-2.147820000	-0.046065000	2.261490000
6	-2.910412000	-0.324694000	3.387086000
6	-3.536859000	-1.548689000	3.524140000
6	-3.382818000	-2.497031000	2.524287000
6	-2.622779000	-2.217909000	1.404318000
1	-3.010351000	0.428029000	4.159606000
1	-3.850964000	-3.469166000	2.621347000
1	-4.133481000	-1.766522000	4.401532000
1	-1.666947000	0.916125000	2.183513000
1	-2.477362000	-2.975300000	0.649252000
6	-1.805383000	-1.029859000	-1.307154000
6	-3.181966000	-1.146383000	-1.448812000
6	-1.026331000	-1.148435000	-2.457209000
6	-3.762648000	-1.366014000	-2.690079000
6	-1.599351000	-1.367954000	-3.694504000
6	-2.976421000	-1.478818000	-3.820816000
1	-3.818426000	-1.051923000	-0.580818000
1	0.049353000	-1.069897000	-2.370032000
1	-4.840239000	-1.447380000	-2.766420000
1	-0.965057000	-1.459005000	-4.567674000
1	-3.427297000	-1.654493000	-4.789531000
6	-1.085884000	1.915390000	-0.007321000
6	-0.622080000	2.997086000	0.758362000
6	-2.252101000	2.141354000	-0.751299000
6	-1.258646000	4.223588000	0.754267000
6	-2.895037000	3.366360000	-0.747005000
6	-2.403721000	4.424182000	-0.000352000
1	0.249147000	2.863915000	1.382612000
1	-2.653138000	1.347338000	-1.360885000
1	-0.860985000	5.027987000	1.361685000
1	-3.790327000	3.494015000	-1.343972000
1	-2.907297000	5.382552000	0.001515000
6	1.954226000	1.479812000	0.058605000
6	2.069903000	2.355149000	-1.015445000
6	2.820850000	1.637314000	1.135941000
6	3.018778000	3.363218000	-1.011997000
6	3.763760000	2.649376000	1.146233000
6	3.868219000	3.517837000	0.071001000
1	1.400300000	2.240731000	-1.857506000
1	2.751541000	0.948865000	1.967880000
1	3.091813000	4.033989000	-1.859064000
1	4.426616000	2.756235000	1.995901000
1	4.609655000	4.306900000	0.076052000
6	2.613170000	-1.612234000	0.084522000
6	3.717783000	-1.026541000	-0.553776000
6	2.822995000	-2.879740000	0.655404000

6	4.952412000	-1.649609000	-0.593075000
6	4.056217000	-3.500365000	0.607692000
6	5.139455000	-2.892072000	-0.010019000
1	3.607200000	-0.070594000	-1.043476000
1	1.985197000	-3.375037000	1.121933000
1	5.776071000	-1.158004000	-1.098131000
1	4.173026000	-4.477333000	1.062906000
1	6.105070000	-3.381061000	-0.045146000
8	-0.087124000	-2.964749000	0.177666000

Structure TS2

6	-1.099048000	-0.483953000	-0.607102000
6	-0.017894000	-1.474087000	-0.855879000
6	1.233835000	-0.731999000	-0.598633000
6	-0.518166000	0.768604000	-0.393134000
6	0.904545000	0.585960000	-0.367142000
6	-0.623095000	-1.665017000	1.089035000
6	-0.415283000	-0.895112000	2.214379000
6	-0.611932000	-1.437845000	3.474237000
6	-1.044521000	-2.750919000	3.607469000
6	-1.265794000	-3.512220000	2.471609000
6	-1.049326000	-2.968955000	1.211452000
1	-0.434753000	-0.833147000	4.356645000
1	-1.602018000	-4.538919000	2.565363000
1	-1.207865000	-3.174098000	4.591075000
1	-0.100506000	0.137398000	2.107998000
1	-1.172561000	-3.557025000	0.307248000
6	-2.518631000	-0.786003000	-0.866590000
6	-3.528802000	-0.373980000	-0.000816000
6	-2.874189000	-1.509619000	-2.003061000
6	-4.856360000	-0.647614000	-0.275774000
6	-4.204138000	-1.781291000	-2.278996000
6	-5.201492000	-1.348394000	-1.420895000
1	-3.264219000	0.160863000	0.901103000
1	-2.087388000	-1.876357000	-2.646240000
1	-5.625493000	-0.316900000	0.411357000
1	-4.461337000	-2.343548000	-3.168564000
1	-6.240820000	-1.564581000	-1.636296000
6	-1.229061000	2.028995000	-0.117528000
6	-0.916666000	2.839578000	0.977001000
6	-2.245975000	2.476348000	-0.966515000
6	-1.583622000	4.029571000	1.212302000
6	-2.921773000	3.659122000	-0.728550000
6	-2.594626000	4.447569000	0.363578000
1	-0.135459000	2.530208000	1.657395000
1	-2.502556000	1.878165000	-1.830055000
1	-1.313211000	4.630931000	2.071838000
1	-3.705846000	3.971285000	-1.407782000
1	-3.119672000	5.376269000	0.548727000
6	1.863583000	1.672798000	-0.072360000
6	1.903699000	2.824243000	-0.854008000
6	2.751151000	1.575768000	0.996577000
6	2.803967000	3.840216000	-0.583282000
6	3.649838000	2.591307000	1.272170000
6	3.682302000	3.729384000	0.482182000
1	1.216920000	2.917014000	-1.684956000
1	2.733841000	0.684064000	1.609418000
1	2.817850000	4.724764000	-1.208071000
1	4.330729000	2.491730000	2.108484000
1	4.386389000	4.523801000	0.695735000
6	2.544475000	-1.358776000	-0.751871000
6	3.662166000	-0.683091000	-1.250542000

6	2.705497000	-2.708904000	-0.420683000
6	4.886919000	-1.314074000	-1.380529000
6	3.929253000	-3.337854000	-0.552619000
6	5.032770000	-2.645649000	-1.027745000
1	3.567618000	0.350228000	-1.551881000
1	1.845001000	-3.260496000	-0.072917000
1	5.732561000	-0.759782000	-1.770198000
1	4.021218000	-4.383337000	-0.283250000
1	5.990473000	-3.140600000	-1.132032000
8	-0.133817000	-2.569071000	-1.440821000

Structure TS3

6	1.127349000	-0.700964000	-0.258478000
6	0.033147000	-1.470936000	-0.971929000
6	-1.238262000	-0.841389000	-0.951125000
6	0.359368000	0.632329000	-0.050926000
6	-0.927320000	0.523344000	-0.440571000
6	2.336063000	-0.639782000	-1.194871000
6	2.647475000	0.487362000	-1.938703000
6	3.707904000	0.479140000	-2.833915000
6	4.466740000	-0.661349000	-3.006763000
6	4.152606000	-1.800830000	-2.282220000
6	3.098513000	-1.789304000	-1.390366000
1	3.934945000	1.375006000	-3.396888000
1	4.728377000	-2.707040000	-2.417140000
1	5.294082000	-0.668105000	-3.704086000
1	2.066781000	1.388347000	-1.829109000
1	2.858705000	-2.690185000	-0.843226000
6	1.456890000	-1.373345000	1.082889000
6	2.719448000	-1.250127000	1.651061000
6	0.486219000	-2.084996000	1.779221000
6	3.000801000	-1.815193000	2.882741000
6	0.768587000	-2.655583000	3.008845000
6	2.027123000	-2.521888000	3.567575000
1	3.491912000	-0.704350000	1.128777000
1	-0.507709000	-2.201945000	1.369065000
1	3.990143000	-1.702741000	3.306694000
1	-0.001991000	-3.210670000	3.527334000
1	2.249671000	-2.969177000	4.527234000
6	0.990662000	1.863371000	0.478083000
6	0.953878000	3.042856000	-0.265598000
6	1.597668000	1.902110000	1.731055000
6	1.506586000	4.213291000	0.218208000
6	2.154840000	3.074115000	2.216049000
6	2.114551000	4.233730000	1.462753000
1	0.474978000	3.039737000	-1.235923000
1	1.617103000	1.014982000	2.345719000
1	1.462103000	5.113867000	-0.380243000
1	2.616155000	3.078911000	3.195109000
1	2.549689000	5.148325000	1.843355000
6	-1.966486000	1.572270000	-0.398913000
6	-2.143422000	2.399128000	0.706778000
6	-2.822218000	1.726472000	-1.486266000
6	-3.135944000	3.362311000	0.716730000
6	-3.807521000	2.697472000	-1.481591000
6	-3.968064000	3.519850000	-0.379307000
1	-1.500111000	2.283529000	1.567906000
1	-2.709429000	1.076432000	-2.344012000
1	-3.260727000	3.992674000	1.587459000
1	-4.457320000	2.806758000	-2.339991000
1	-4.743156000	4.274790000	-0.370816000
6	-2.476684000	-1.564485000	-0.516568000

6	-3.045972000	-1.282050000	0.725463000
6	-3.090537000	-2.535317000	-1.304170000
6	-4.172287000	-1.953410000	1.165724000
6	-4.205767000	-3.222917000	-0.856735000
6	-4.754621000	-2.933408000	0.379607000
1	-2.600037000	-0.525823000	1.356523000
1	-2.701540000	-2.753466000	-2.290414000
1	-4.594356000	-1.710693000	2.132368000
1	-4.656737000	-3.976526000	-1.489013000
1	-5.635158000	-3.459334000	0.723938000
8	0.153279000	-2.422757000	-1.802820000
1	-0.900483000	-1.722516000	-2.130643000

Structure 3

6	1.120510000	-0.734232000	-0.174979000
6	-0.000780000	-1.769423000	-0.421142000
6	-1.293197000	-1.036227000	-0.776451000
6	0.309474000	0.562835000	-0.061202000
6	-0.979874000	0.387539000	-0.379804000
6	1.986192000	-0.818861000	-1.440042000
6	1.927384000	0.130770000	-2.448299000
6	2.680214000	-0.009945000	-3.605330000
6	3.494512000	-1.112297000	-3.775958000
6	3.546240000	-2.078802000	-2.782718000
6	2.799657000	-1.934710000	-1.629813000
1	2.624016000	0.749823000	-4.373943000
1	4.169804000	-2.954155000	-2.909081000
1	4.082194000	-1.223979000	-4.677575000
1	1.289835000	0.993676000	-2.340214000
1	2.835986000	-2.701517000	-0.868949000
6	1.907741000	-1.042045000	1.094890000
6	3.245517000	-0.687822000	1.215489000
6	1.274801000	-1.608372000	2.195832000
6	3.931284000	-0.889924000	2.401005000
6	1.957335000	-1.812133000	3.382455000
6	3.290056000	-1.452717000	3.490532000
1	3.759088000	-0.240257000	0.376393000
1	0.235997000	-1.903582000	2.133798000
1	4.972235000	-0.602603000	2.471555000
1	1.444765000	-2.259982000	4.223690000
1	3.825887000	-1.614774000	4.416504000
6	0.921821000	1.864261000	0.312102000
6	0.896833000	2.936103000	-0.577157000
6	1.494101000	2.067552000	1.565909000
6	1.436101000	4.162763000	-0.235759000
6	2.029846000	3.296826000	1.910904000
6	2.008919000	4.347655000	1.010929000
1	0.430469000	2.814413000	-1.545311000
1	1.507421000	1.264549000	2.287773000
1	1.403855000	4.978222000	-0.946335000
1	2.463572000	3.431432000	2.893174000
1	2.430773000	5.306739000	1.281046000
6	-2.044120000	1.412517000	-0.407723000
6	-2.196240000	2.348949000	0.611225000
6	-2.947872000	1.438362000	-1.467113000
6	-3.208118000	3.290409000	0.562413000
6	-3.953827000	2.386219000	-1.522502000
6	-4.087842000	3.317152000	-0.506934000
1	-1.517653000	2.336417000	1.452378000
1	-2.863827000	0.709388000	-2.262397000
1	-3.311348000	4.005912000	1.367649000
1	-4.639900000	2.392027000	-2.359270000

1	-4.878662000	4.054613000	-0.544097000
6	-2.501748000	-1.681396000	-0.145707000
6	-2.867525000	-1.395945000	1.163444000
6	-3.237086000	-2.621540000	-0.853275000
6	-3.946787000	-2.033570000	1.749718000
6	-4.316369000	-3.262365000	-0.269657000
6	-4.675026000	-2.969533000	1.034726000
1	-2.310193000	-0.660056000	1.728807000
1	-2.957564000	-2.860080000	-1.871988000
1	-4.221594000	-1.796066000	2.769134000
1	-4.878138000	-3.993244000	-0.836432000
1	-5.519866000	-3.467181000	1.492198000
8	0.125348000	-2.954345000	-0.351659000
1	-1.392726000	-1.113279000	-1.865279000

Coordinates from computations at CAM-B3LYP/Def2SVP level.

Structure B×MeOH

6	0.854986000	-0.970951000	-0.031004000
6	-0.655553000	-1.164329000	0.003003000
6	-1.308459000	0.022845000	-0.037011000
6	0.962786000	0.563438000	-0.022358000
6	-0.286094000	1.093824000	-0.019590000
6	1.346584000	-1.629025000	-1.331247000
6	1.746341000	-0.886186000	-2.443518000
6	2.124931000	-1.515852000	-3.629043000
6	2.107828000	-2.901672000	-3.726160000
6	1.701500000	-3.655070000	-2.626254000
6	1.323531000	-3.026596000	-1.445847000
1	2.438641000	-0.909106000	-4.481472000
1	1.676258000	-4.745511000	-2.687918000
1	2.408191000	-3.394956000	-4.653276000
1	1.769816000	0.199797000	-2.393405000
1	0.993229000	-3.626084000	-0.597973000
6	1.492676000	-1.570363000	1.232110000
6	2.737072000	-2.203248000	1.211040000
6	0.845112000	-1.426855000	2.464101000
6	3.317795000	-2.678919000	2.385551000
6	1.422040000	-1.899136000	3.637509000
6	2.663878000	-2.530282000	3.604005000
1	3.270197000	-2.318107000	0.267213000
1	-0.126667000	-0.930888000	2.504788000
1	4.293463000	-3.168365000	2.342915000
1	0.895251000	-1.775741000	4.586459000
1	3.117540000	-2.905241000	4.524011000
6	2.230386000	1.333038000	-0.069091000
6	2.404726000	2.337284000	-1.035503000
6	3.274265000	1.121690000	0.843578000
6	3.569683000	3.093453000	-1.092799000
6	4.443099000	1.876796000	0.784507000
6	4.599003000	2.864346000	-0.183053000
1	1.605421000	2.527352000	-1.754203000
1	3.166405000	0.371549000	1.624893000
1	3.674468000	3.866831000	-1.857146000
1	5.237565000	1.692368000	1.511336000
1	5.516736000	3.454904000	-0.227108000
6	-0.633041000	2.535062000	0.011519000
6	-0.109449000	3.378118000	0.999272000
6	-1.502466000	3.082290000	-0.940609000
6	-0.438326000	4.729791000	1.029003000
6	-1.825859000	4.435552000	-0.915301000
6	-1.295751000	5.264329000	0.070449000

1	0.565150000	2.962930000	1.749959000
1	-1.923996000	2.438925000	-1.715369000
1	-0.019704000	5.371089000	1.807842000
1	-2.499291000	4.845362000	-1.671426000
1	-1.552290000	6.325765000	0.092716000
6	-2.774699000	0.205079000	-0.042883000
6	-3.424562000	0.985816000	0.924082000
6	-3.561424000	-0.421795000	-1.021194000
6	-4.809661000	1.121543000	0.923410000
6	-4.949228000	-0.289997000	-1.021456000
6	-5.579674000	0.480962000	-0.045850000
1	-2.831039000	1.487756000	1.690242000
1	-3.069120000	-1.019809000	-1.791316000
1	-5.293179000	1.731744000	1.689383000
1	-5.540808000	-0.782253000	-1.797177000
1	-6.666282000	0.590000000	-0.046924000
8	-1.117377000	-2.402753000	0.106790000
1	-4.194685000	-2.040651000	0.701525000
1	-2.072662000	-2.456134000	0.358811000
6	-4.259195000	-3.949164000	0.258518000
1	-4.443036000	-3.802092000	-0.819901000
1	-3.576055000	-4.800517000	0.378860000
1	-5.213710000	-4.201966000	0.749868000
8	-3.649434000	-2.825228000	0.856017000

Structure 3×MeOH

6	1.109399000	-0.547214000	0.199559000
6	-0.082876000	-1.529246000	0.184900000
6	-1.339837000	-0.824636000	-0.308089000
6	0.413114000	0.782515000	-0.132702000
6	-0.899291000	0.619331000	-0.404697000
6	2.029055000	-1.073854000	-0.915717000
6	2.065927000	-0.499511000	-2.186241000
6	2.849915000	-1.050718000	-3.199876000
6	3.601240000	-2.194712000	-2.960990000
6	3.557721000	-2.789216000	-1.700244000
6	2.778997000	-2.236992000	-0.691021000
1	2.867137000	-0.577187000	-4.183828000
1	4.134332000	-3.695249000	-1.501370000
1	4.215984000	-2.626880000	-3.753462000
1	1.474957000	0.388673000	-2.398482000
1	2.737722000	-2.720649000	0.285064000
6	1.792854000	-0.520264000	1.569368000
6	3.158345000	-0.250804000	1.695344000
6	1.039757000	-0.687819000	2.735837000
6	3.753990000	-0.150752000	2.949639000
6	1.632807000	-0.588830000	3.991260000
6	2.994059000	-0.319446000	4.103602000
1	3.765773000	-0.108130000	0.801029000
1	-0.029402000	-0.900411000	2.674300000
1	4.822507000	0.063220000	3.023200000
1	1.024438000	-0.728664000	4.887324000
1	3.461578000	-0.244521000	5.087706000
6	1.144514000	2.079247000	-0.191690000
6	1.193502000	2.810984000	-1.386335000
6	1.762900000	2.626371000	0.940898000
6	1.851477000	4.033832000	-1.455405000
6	2.418625000	3.853260000	0.873257000
6	2.471511000	4.559145000	-0.324683000
1	0.691684000	2.421942000	-2.274214000
1	1.714416000	2.099745000	1.893118000
1	1.875615000	4.582013000	-2.399685000

1	2.888915000	4.261006000	1.770754000
1	2.988823000	5.519586000	-0.376077000
6	-1.880681000	1.665550000	-0.778317000
6	-1.907232000	2.919660000	-0.154006000
6	-2.837256000	1.395944000	-1.766089000
6	-2.847492000	3.876728000	-0.519406000
6	-3.771291000	2.357028000	-2.139175000
6	-3.779486000	3.602450000	-1.517485000
1	-1.187745000	3.144326000	0.633818000
1	-2.850307000	0.419832000	-2.254544000
1	-2.853833000	4.845957000	-0.016046000
1	-4.502570000	2.126895000	-2.916942000
1	-4.516703000	4.355549000	-1.803900000
6	-2.539475000	-1.109802000	0.578324000
6	-2.787577000	-0.343399000	1.720919000
6	-3.389943000	-2.179155000	0.284245000
6	-3.864225000	-0.637792000	2.553069000
6	-4.465997000	-2.472824000	1.117981000
6	-4.707409000	-1.704519000	2.253672000
1	-2.139632000	0.503483000	1.957005000
1	-3.196704000	-2.791348000	-0.599452000
1	-4.047323000	-0.025481000	3.438854000
1	-5.122743000	-3.311045000	0.874709000
1	-5.553904000	-1.934731000	2.904337000
8	-0.007172000	-2.695062000	0.475719000
1	-1.540340000	-1.263513000	-1.301160000
1	-1.023837000	-3.690290000	-0.811609000
6	-0.497035000	-4.313387000	-2.580828000
1	0.446010000	-3.737471000	-2.624965000
1	-0.243306000	-5.361541000	-2.333705000
1	-0.940035000	-4.310042000	-3.587927000
8	-1.429970000	-3.760939000	-1.691609000

Structure TS4

6	1.159222000	-0.606165000	0.136070000
6	-0.043297000	-1.573913000	0.056165000
6	-1.255582000	-0.858225000	-0.167907000
6	0.463163000	0.754966000	0.002687000
6	-0.867577000	0.584952000	-0.177620000
6	2.073555000	-0.968092000	-1.040005000
6	2.216483000	-0.142530000	-2.157730000
6	2.989132000	-0.538841000	-3.250166000
6	3.632942000	-1.770558000	-3.245860000
6	3.496795000	-2.605490000	-2.137348000
6	2.726456000	-2.210360000	-1.049804000
1	3.088723000	0.130308000	-4.107795000
1	3.995652000	-3.577213000	-2.119118000
1	4.241585000	-2.079465000	-4.098628000
1	1.725275000	0.827429000	-2.183293000
1	2.609376000	-2.879390000	-0.198229000
6	1.832486000	-0.764412000	1.506526000
6	3.218281000	-0.738999000	1.670303000
6	1.031445000	-0.873117000	2.649585000
6	3.788592000	-0.820976000	2.939527000
6	1.597800000	-0.958565000	3.916510000
6	2.982820000	-0.933429000	4.067538000
1	3.866220000	-0.639070000	0.799469000
1	-0.056294000	-0.877462000	2.549756000
1	4.875646000	-0.793463000	3.043189000
1	0.951408000	-1.044785000	4.792659000
1	3.430436000	-1.000355000	5.061423000
6	1.163535000	2.065585000	0.051929000

6	0.985667000	3.003097000	-0.977692000
6	1.995585000	2.427566000	1.121910000
6	1.613219000	4.243651000	-0.946071000
6	2.626766000	3.668342000	1.152793000
6	2.442028000	4.582281000	0.119993000
1	0.338087000	2.753320000	-1.819563000
1	2.138805000	1.740532000	1.953886000
1	1.453165000	4.950436000	-1.763457000
1	3.265428000	3.923369000	2.001592000
1	2.938226000	5.554848000	0.147062000
6	-1.844921000	1.694276000	-0.334719000
6	-2.165566000	2.521697000	0.744432000
6	-2.454279000	1.941313000	-1.570876000
6	-3.073215000	3.567172000	0.593547000
6	-3.357549000	2.988044000	-1.725131000
6	-3.671886000	3.804110000	-0.640187000
1	-1.693290000	2.341415000	1.711855000
1	-2.208370000	1.305370000	-2.425340000
1	-3.312487000	4.203050000	1.448737000
1	-3.818101000	3.169941000	-2.698844000
1	-4.381817000	4.625560000	-0.758321000
6	-2.566769000	-1.357348000	0.370417000
6	-2.604445000	-2.331003000	1.381314000
6	-3.792783000	-0.881470000	-0.116426000
6	-3.813078000	-2.794623000	1.891263000
6	-5.001267000	-1.338847000	0.400312000
6	-5.020456000	-2.298201000	1.408180000
1	-1.670887000	-2.743249000	1.765842000
1	-3.806612000	-0.139386000	-0.913432000
1	-3.807635000	-3.550996000	2.679668000
1	-5.938565000	-0.942553000	0.002899000
1	-5.969018000	-2.660025000	1.810669000
8	0.094704000	-2.818174000	0.030959000
1	-1.400613000	-1.743210000	-1.438181000
1	-0.823944000	-3.137444000	-1.096759000
6	-0.592665000	-2.850976000	-3.109125000
1	0.342562000	-2.281840000	-3.000863000
1	-0.360574000	-3.902599000	-3.322239000
1	-1.189363000	-2.440217000	-3.933201000
8	-1.380560000	-2.791618000	-1.918140000

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