

Electronic Supplementary Information

for
NJC

Selective recognition of “solvent” molecules in solution and the solid state by 1,4-dimethoxypillar[5]arene driven by attractive forces**

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1. Association constant determination for the complexation of 1,4-dimethoxypillar[5]arene (DMP[5]A) with acetonitrile, dichloromethane, ethyl acetate, acetone, and hexane

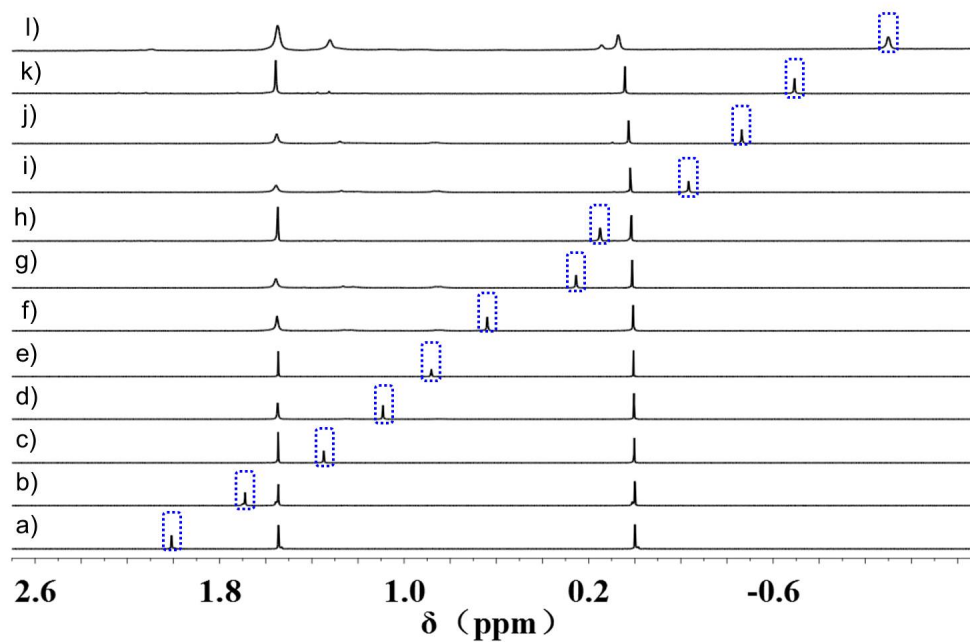


Figure S1. Partial ^1H NMR spectra (300 MHz, CDCl_3 , 298 K) of acetonitrile at the concentration of 5 mM upon addition of DMP[5]A: (a) 0 mM; (b) 4 mM; (c) 8 mM; (d) 12 mM; (e) 16 mM; (f) 20 mM; (g) 30 mM; (h) 40 mM; (i) 50 mM; (j) 70 mM; (k) 100 mM; (l) 150 mM. This set of data was used for the non-linear curve-fitting.

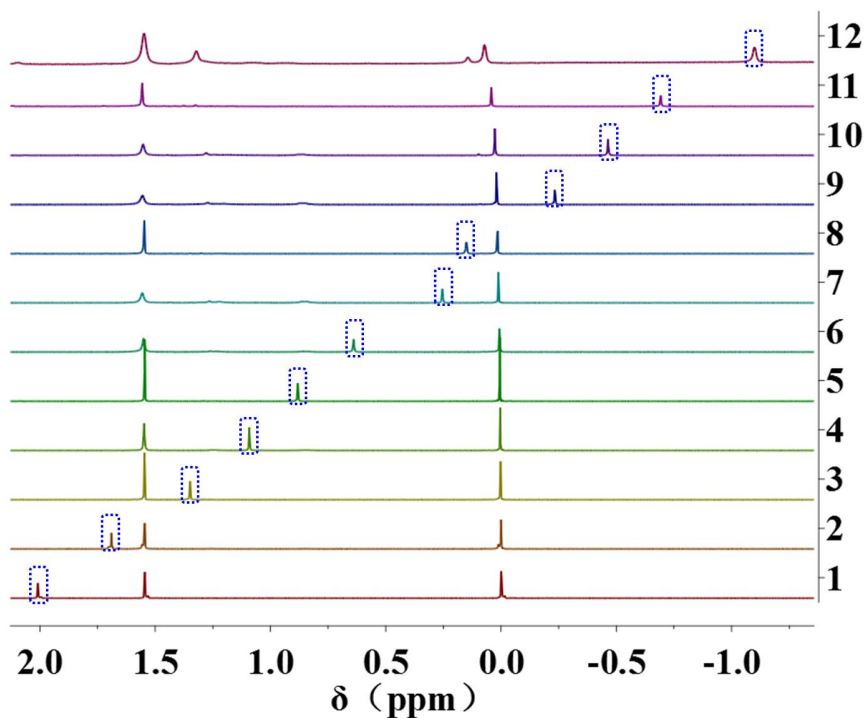


Figure S2. Partial ^1H NMR spectra (300 MHz, CDCl_3 , 298 K) of acetonitrile at the concentration of 5 mM upon addition of DMP[5]A: (1) 0 mM; (2) 4 mM; (3) 8 mM; (4) 12 mM; (5) 16 mM; (6) 20 mM; (7) 30 mM; (8) 40 mM; (9) 50 mM; (10) 70 mM; (11) 100 mM; (12) 150 mM. Repetition of the experimental data in Figure S1.

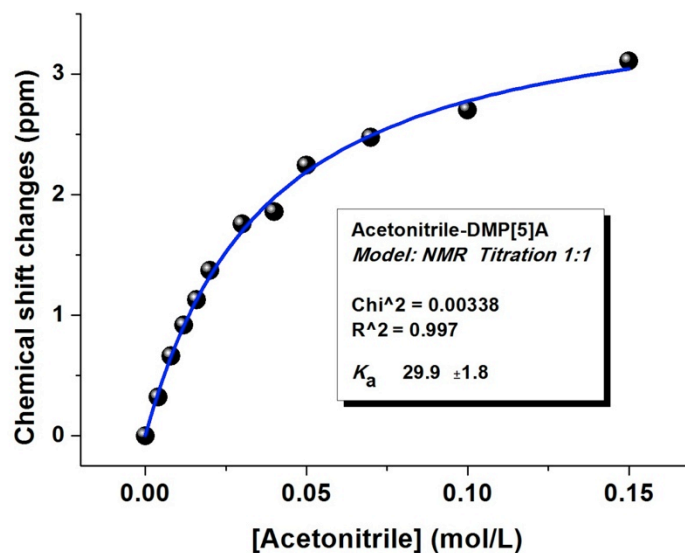


Figure S3. The non-linear curve-fitting (NMR titrations) for the complexation of acetonitrile (5 mM) with DMP[5]A in CDCl_3 at 298 K (Figure S2). The concentration of DMP[5]A was 0, 4, 8, 12, 16, 20, 30, 40, 50, 70, 100 and 150 mM, respectively. Association constant (K_a) is calculated to be 29.9 M^{-1} .

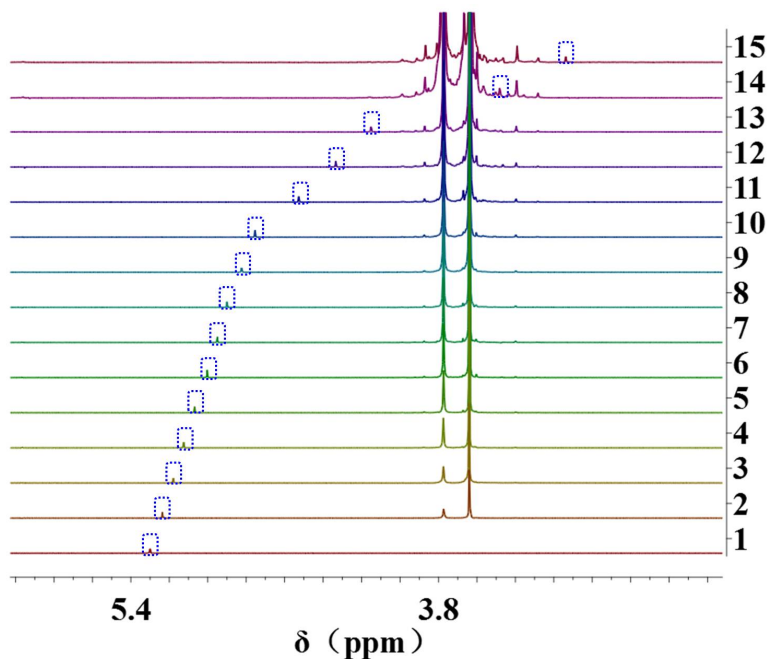


Figure S4. Partial ^1H NMR spectra (300 MHz, CDCl_3 , 298 K) of dichloromethane at the concentration of 7.8 mM upon addition of DMP[5]A: (1) 0 mM; (2) 2 mM; (3) 4 mM; (4) 6 mM; (5) 8 mM; (6) 10 mM; (7) 12 mM; (8) 14 mM; (9) 17 mM; (10) 20 mM; (11) 30 mM; (12) 40 mM; (13) 50 mM; (14) 100 mM; (15) 140 mM. Repetition of the experiments in Fig. 4.

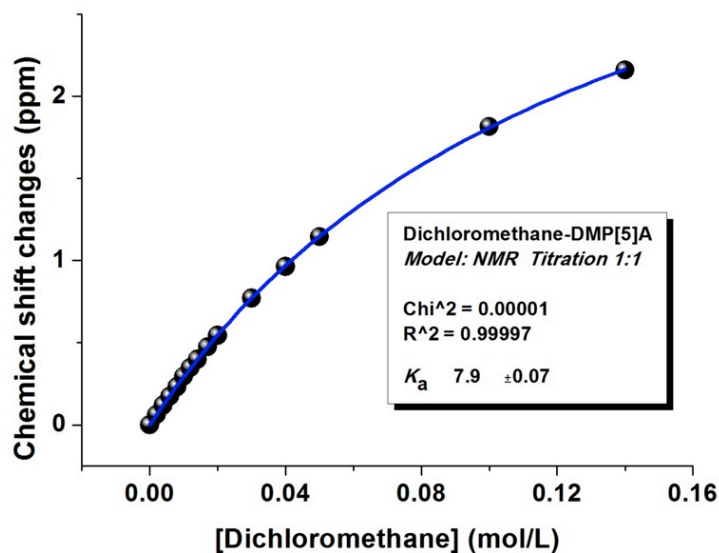


Figure S5. The non-linear curve-fitting (NMR titrations) for the complexation of dichloromethane (7.8 mM) with DMP[5]A in CDCl_3 at 298 K (Figure S4). The concentration of DMP[5]A was 0, 2, 4, 6, 8, 10, 12, 14, 17, 20, 30, 40, 50, 100 and 140 mM, respectively. Association constant (K_a) is calculated to be 7.9 M^{-1} .

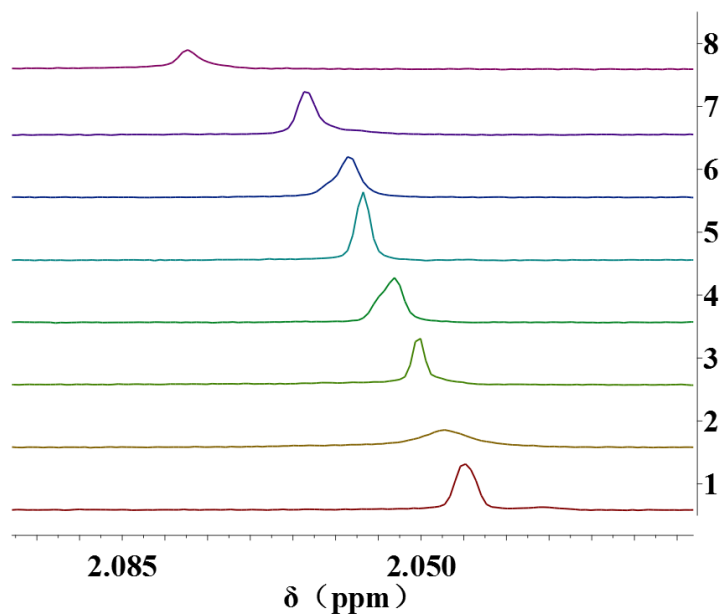


Figure S6. Partial ^1H NMR spectra (300 MHz, CDCl_3 , 298 K) of ethyl acetate at the concentration of 2.5 mM upon addition of DMP[5]A: (1) 0 mM; (2) 8 mM; (3) 16 mM; (4) 30 mM; (5) 40 mM; (6) 50 mM; (7) 70 mM; (8) 100 mM.

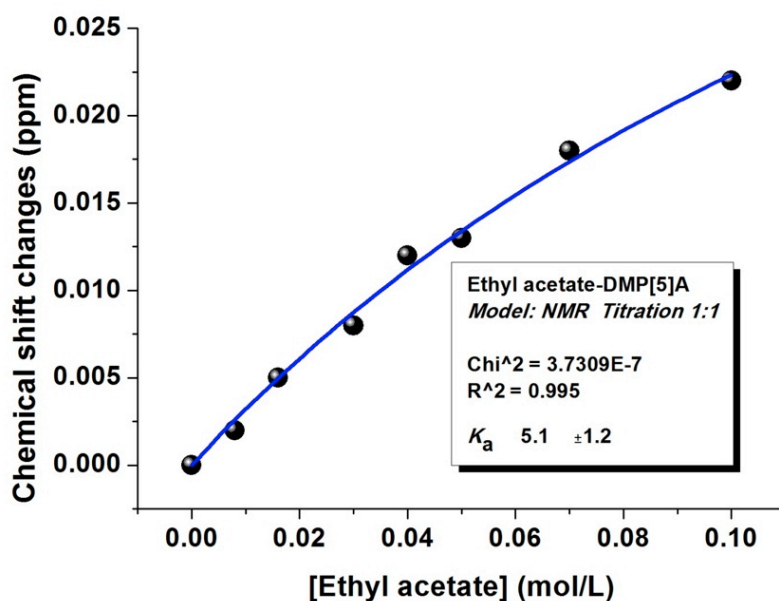


Figure S7. The non-linear curve-fitting (NMR titrations) for the complexation of ethyl acetate (2.5 mM) with DMP[5]A in CDCl_3 at 298 K (Figure S6). The concentration of DMP[5]A was 0, 8, 16, 30, 40, 50, 70 and 100 mM, respectively. Association constant (K_a) is calculated to be 5.1 M^{-1} .

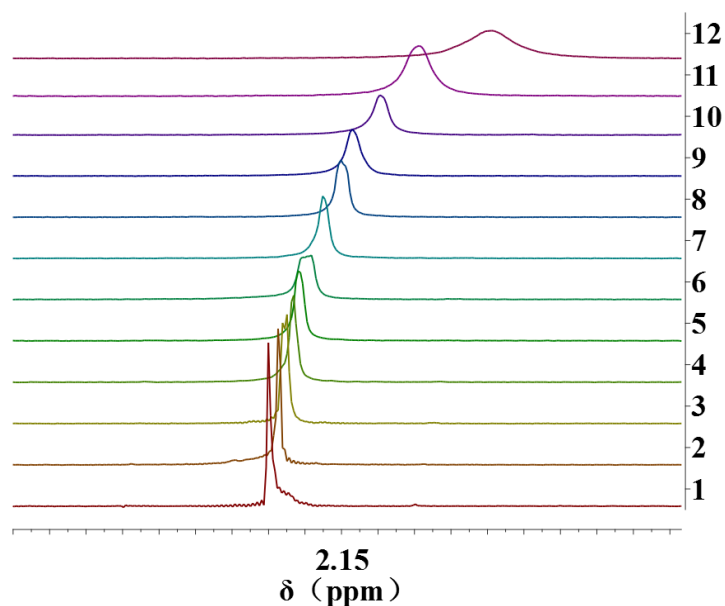


Figure S8. Partial ^1H NMR spectra (300 MHz, CDCl_3 , 298 K) of acetone at the concentration of 5 mM upon addition of DMP[5]A: (1) 0 mM; (2) 4 mM; (3) 8 mM; (4) 12 mM; (5) 16 mM; (6) 20 mM; (7) 30 mM; (8) 40 mM; (9) 50 mM; (10) 70 mM; (11) 100 mM; (12) 150 mM.

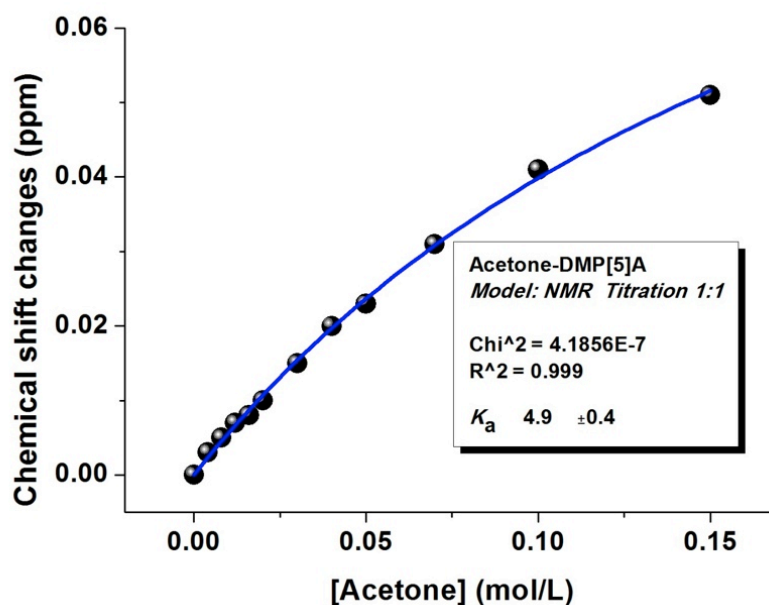


Figure S9. The non-linear curve-fitting (NMR titrations) for the complexation of acetone (5 mM) with DMP[5]A in CDCl_3 at 298 K (Figure S8). The concentration of DMP[5]A was 0, 4, 8, 12, 16, 20, 30, 40, 50, 70, 100 and 150 mM, respectively. Association constant (K_a) is calculated to be 4.9 M^{-1} .

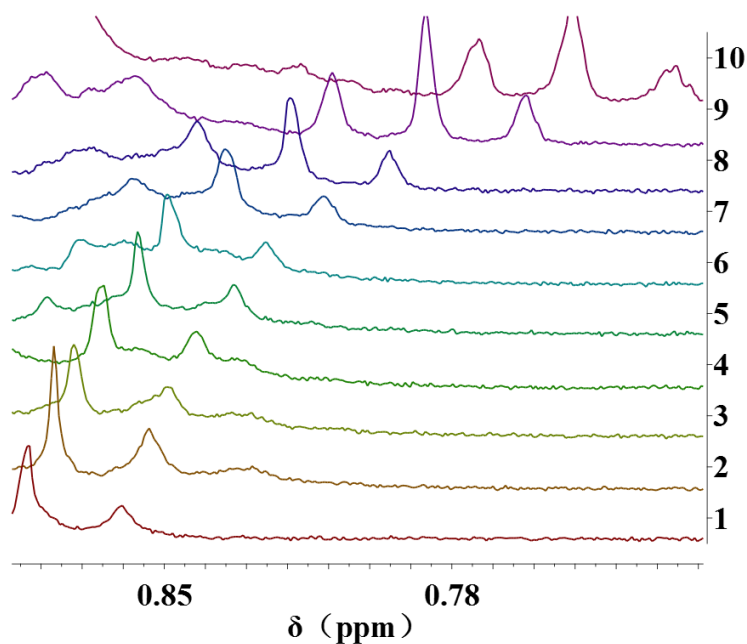


Figure S10. Partial ^1H NMR spectra (300 MHz, CDCl_3 , 298 K) of hexane at the concentration of 2.5 mM upon addition of DMP[5]A: (1) 0 mM; (2) 4 mM; (3) 8 mM; (4) 12 mM; (5) 16 mM; (6) 20 mM; (7) 30 mM; (8) 40 mM; (9) 70 mM; (10) 100 mM.

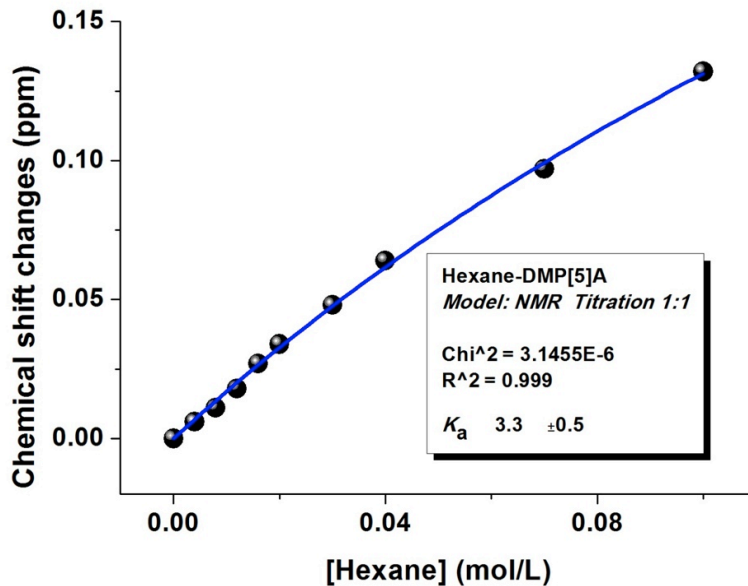


Figure S11. The non-linear curve-fitting (NMR titrations) for the complexation of hexane (2.5 mM) with DMP[5]A in CDCl_3 at 298 K (Figure S10). The concentration of DMP[5]A was 0, 4, 8, 12, 16, 20, 30, 40, 70, and 100 mM respectively. Association constant (K_a) is calculated to be 3.3 M^{-1} .

2. X-ray crystal data analysis

The size of DMP[5]A was estimated according to the reference.^[S1]

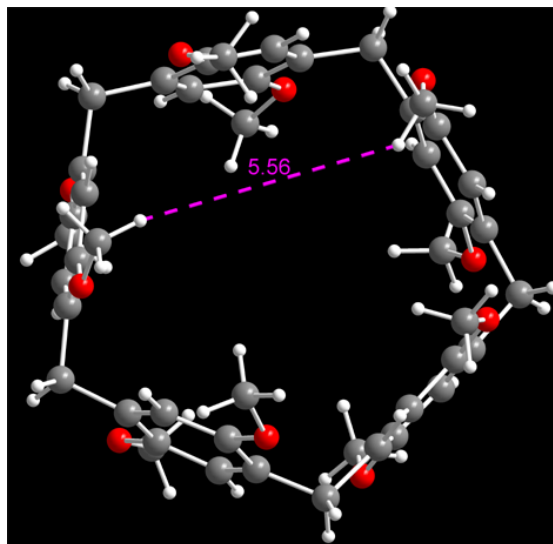


Figure S12. Crystal structure of DMP[5]A. Oxygen atoms are red, carbon atoms are medium grey and hydrogen atoms are white. Dashes represent the shortest distance of two hydrogens (purple). Size parameter: H \cdots H distance (Å), 5.56.

The smallest size of DMP[5]A (Å): $5.56 - 2 \times \text{vander Waals Radium of hydrogen}$
 $= 5.56 - 2 \times 1.10 = 3.36$.

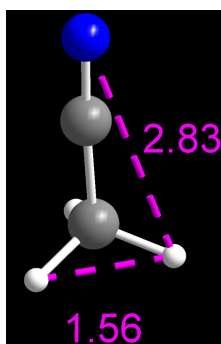


Figure S13. Crystal structure of acetonitrile. Nitrogen atom is blue, carbon atoms are medium grey and hydrogen atoms are white. Dashes represent the longest length and width of acetonitrile (purple). Size parameter: N \cdots H distance (Å), 2.83; H \cdots H distance (Å), 1.56.

The longest length of acetonitrile (Å): $2.83 + \text{vander Waals Radium of hydrogen} + \text{vander Waals Radium of nitrogen} = 2.83 + 1.10 + 1.5 = 5.43$.

The longest width of acetonitrile (Å): $1.56 + 2 \times \text{vander Waals Radium of hydrogen} = 1.56 + 2 \times 1.10 = 3.76$.

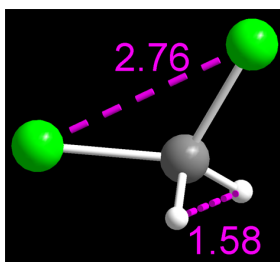


Figure S14. Crystal structure of dichloromethane. Chlorine atoms are green, carbon atoms are medium grey and hydrogen atoms are white. Dashes represent the longest length and width of dichloromethane (purple). Size parameter: Cl \cdots Cl distance (Å), 2.76; H \cdots H distance (Å), 1.58.

The longest length of dichloromethane (Å): $2.76 + 2 \times \text{vander Waals Radium of chlorine} = 2.76 + 2 \times 1.80 = 6.36$.

The longest width of dichloromethane (Å): $1.58 + 2 \times \text{vander Waals Radium of hydrogen} = 1.58 + 2 \times 1.10 = 3.78$.

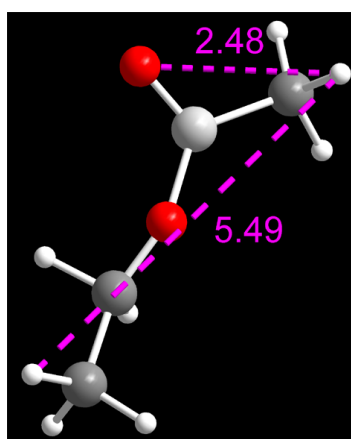


Figure S15. Crystal structure of ethyl acetate. Oxygen atoms are red, carbon atoms are medium grey and hydrogen atoms are white. Dashes represent the longest length and width of ethyl acetate (purple). Size parameter: H \cdots H distance (Å), 5.49; H \cdots O distance (Å), 2.48.

The longest length of ethyl acetate (Å): $5.49 + 2 \times \text{vander Waals Radium of hydrogen} = 5.49 + 2 \times 1.10 = 7.69$.

The longest width of ethyl acetate (Å): $2.48 + \text{vander Waals Radium of hydrogen} + \text{vander Waals Radium of oxygen} = 2.48 + 1.40 + 1.1 = 4.98$.

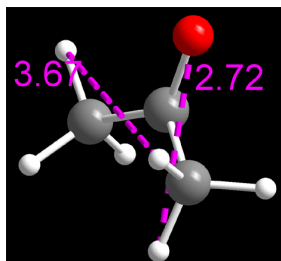


Figure S16. Crystal structure of acetone. Oxygen atoms are red, carbon atoms are medium grey and hydrogen atoms are white. Dashes represent the longest length and width of acetone (purple). Size parameter: H \cdots H distance (Å), 3.67; H \cdots O distance (Å), 2.72.

The longest length of acetone (Å): $3.67 + 2 \times \text{vander Waals Radium of hydrogen} = 3.67 + 2 \times 1.10 = 5.87$.

The longest width of acetone (Å): $2.72 + \text{vander Waals Radium of hydrogen} + \text{vander Waals Radium of oxygen} = 2.72 + 1.40 + 1.1 = 5.22$.

3. MALDI-TOF-MS spectra of acetonitrileCDMP[5]A

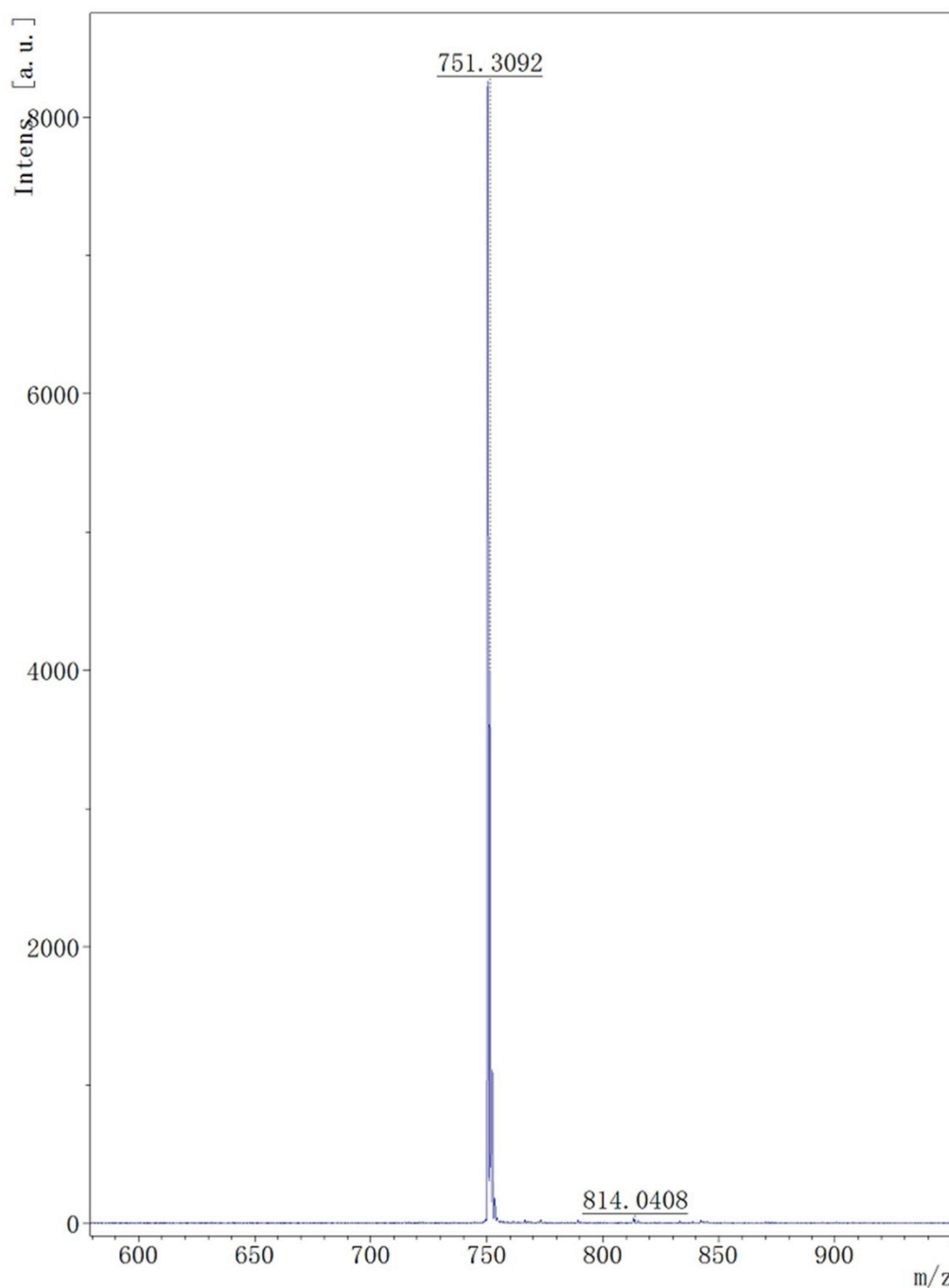


Figure S17. MS (MALDI-TOF) of acetonitrileCDMP[5]A. Peak at m/z 814.0408 (100%) corresponds to $[M + \text{CH}_3\text{CN} + \text{Na}]^+$, peak at m/z 751.3092 (100%) corresponding to $[M + \text{H}]^+$.

4. Computational calculation data for the host-guest complexation of DMP[5]A and small organic molecules

Acetonitrile⊂DMP[5]A:

C	-2.08709800	4.53744900	0.08990700
C	-2.88043000	3.23989100	0.10093000
C	-0.58582700	4.29663500	0.08552100
C	-3.21231800	2.60117900	-1.09827400
C	-3.26491600	2.63176000	1.30708000
C	0.12367000	4.20210000	1.28624600
C	0.11605100	4.12006100	-1.11904400
H	-2.89750100	3.07223600	-2.02041800
C	-3.89821900	1.38320500	-1.11407700
C	-3.95279000	1.41461000	1.29209500
O	-2.92297900	3.29855300	2.46451900
H	-0.43128000	4.32508300	2.20813000
C	1.49393800	3.92494500	1.30621900
C	1.48639500	3.84690400	-1.09878100
O	-0.61865900	4.23880800	-2.27634500
C	-4.27330100	0.76964700	0.09357100
O	-4.24946500	0.72308300	-2.26893800
H	-4.23342400	0.92418700	2.21600200
C	-3.36294400	2.75949600	3.69750100
C	2.19387700	3.73887200	0.10285800
O	2.23157800	3.81348400	2.46632900
H	2.03364400	3.68876200	-2.01915900
C	0.03587100	3.99886600	-3.51315900
C	-4.96707400	-0.58314700	0.10383700
C	-3.82497000	1.26860600	-3.50907300

H	-4.45678200	2.67509700	3.73786500
H	-3.02960000	3.45559900	4.46966100
H	-2.92559600	1.77099500	3.89117800
C	3.67330500	3.38695900	0.09673700
C	1.58003300	4.07249700	3.69621900
H	0.85865000	4.70594500	-3.68032400
H	-0.72047700	4.14662700	-4.28616400
H	0.41858000	2.97289800	-3.57440600
H	-5.60618500	-0.65029500	0.98738400
H	-5.60575200	-0.66684700	-0.77898200
C	-3.97719200	-1.73751900	0.11144000
H	-4.24045400	2.27089900	-3.67500100
H	-4.20666300	0.59553800	-4.27895000
H	-2.73107300	1.31181700	-3.57715000
H	4.14074800	3.82765000	-0.78734300
H	4.15050300	3.82002800	0.97897900
C	3.90884800	1.88477400	0.09041100
H	1.16379300	5.08780400	3.73078300
H	2.34269600	3.97259300	4.47100200
H	0.77284900	3.35377900	3.89085200
C	-3.47867800	-2.25114700	-1.08973200
C	-3.50857500	-2.28736600	1.31575100
C	4.02548700	1.17714600	1.29097900
C	3.97318700	1.16579400	-1.11548700
H	-3.83700600	-1.81009500	-2.01096800
C	-2.52816500	-3.27551200	-1.10927900
C	-2.56126900	-3.31534500	1.29707300
O	-4.03012200	-1.75387000	2.47581900
H	3.95992500	1.74078100	2.21343700
C	4.18837500	-0.21128700	1.30887500

C	4.13819000	-0.22206900	-1.09627500
O	3.87005200	1.90330100	-2.27262800
C	-2.05262100	-3.81925600	0.09612400
O	-2.01089400	-3.81083400	-2.26655900
H	-2.17543600	-3.73238600	2.21912600
C	-3.64443500	-2.33660200	3.70700800
C	4.24192500	-0.93119800	0.10424300
O	4.29853800	-0.94979300	2.46834700
H	4.16501400	-0.78986200	-2.01725800
C	3.85211600	1.20851000	-3.51046700
C	-0.97777800	-4.89495800	0.10105700
C	-2.40891400	-3.24116200	-3.50439800
H	-3.90177500	-3.40292200	3.75118100
H	-4.19759800	-1.80315200	4.48248500
H	-2.56761900	-2.22601200	3.89206000
C	4.36296300	-2.44716100	0.09562700
C	4.32681500	-0.25317700	3.70052300
H	4.78079300	0.64686100	-3.67414400
H	3.76096100	1.97444300	-4.28276900
H	2.99667400	0.52525600	-3.57651800
H	-1.09641400	-5.52569700	-0.78342700
H	-1.10790500	-5.52655000	0.98298500
C	0.42560200	-4.30927900	0.10723600
H	-3.49100400	-3.33316000	-3.66384400
H	-1.88755500	-3.80896800	-4.27719600
H	-2.11874000	-2.18575400	-3.57442600
H	4.92247200	-2.76904700	0.97710700
H	4.92575600	-2.75458000	-0.78932200
C	3.00603200	-3.13334500	0.09011700
H	5.16107400	0.45893800	3.74675300

H	4.46076100	-1.01093100	4.47499700
H	3.38983000	0.28880300	3.88559100
C	1.06389300	-3.98468000	-1.09449500
C	1.10030500	-4.04659600	1.31078000
C	2.37378900	-3.46957600	1.29070000
C	2.33504600	-3.40366900	-1.11483100
H	0.52891200	-4.18043400	-2.01485500
O	0.43591000	-4.38525500	2.47102400
H	2.89415500	-3.24156100	2.21266900
O	3.00059500	-3.07079000	-2.27198300
C	1.11483800	-4.21275300	3.70143200
C	2.33207700	-3.26451000	-3.50940400
H	2.04719800	-4.79123700	3.73678300
H	0.43783200	-4.57865000	4.47582800
H	1.34724000	-3.15720300	3.89588100
H	2.08327900	-4.32070200	-3.67500000
H	3.03170700	-2.94032000	-4.28195200
H	1.41880000	-2.66053200	-3.57321800
H	-0.92861800	0.48773800	-0.23301800
H	0.85269800	0.54471500	-0.21754600
H	0.01164500	-1.02760200	-0.22225200
C	-0.00633200	-0.00211800	-2.05130400
C	-0.01823700	0.00072400	-0.59254500
N	0.00137400	-0.00439000	-3.21403300
H	-2.36156100	5.11506800	-0.79634200
H	-2.35149300	5.12843100	0.96995400

DichloromethaneCDMP[5]A:

C	-4.89847200	-0.63224800	0.75784900
C	-3.89432300	-1.77374200	0.70348300
C	-4.23454300	0.72917800	0.61553000
C	-3.15870300	-2.12264500	1.84098700
C	-3.65096300	-2.47828100	-0.48621600
C	-4.02138900	1.29293200	-0.64825100
C	-3.78916300	1.44057100	1.74088400
H	-3.35675200	-1.57357100	2.75279600
C	-2.18409800	-3.12156000	1.80354400
C	-2.66633400	-3.47323500	-0.52471900
O	-4.40939000	-2.11795600	-1.57941700
H	-4.37587700	0.74333300	-1.51286800
C	-3.36860200	2.52193400	-0.80181500
C	-3.13092300	2.66338300	1.58708500
O	-4.03721900	0.86296300	2.96921400
C	-1.90588300	-3.79710200	0.60258300
O	-1.45180100	-3.50978900	2.90243800
H	-2.45328700	-3.99999400	-1.44712500
C	-4.39763200	-2.97177900	-2.71309000
C	-2.89973500	3.21804000	0.32586900
O	-3.14857100	3.12022400	-2.02141300
H	-2.75809300	3.20430300	2.44778700
C	-3.72454000	1.60978200	4.13147300
C	-0.79304600	-4.83145000	0.52517900
C	-1.70639000	-2.86168400	4.13538900
H	-3.42861200	-2.95832000	-3.22581300
H	-5.15888000	-2.58221800	-3.39163200
H	-4.64893300	-4.00462600	-2.43990000

C	-2.13041300	4.52319400	0.18746200
C	-3.73280800	2.53298100	-3.17272700
H	-2.64612300	1.79500300	4.22221900
H	-4.05646600	1.00596200	4.97832600
H	-4.25038600	2.57317600	4.14807600
H	-0.81929900	-5.45667300	1.42248700
H	-0.97646500	-5.47851100	-0.33692100
C	0.59444300	-4.21791600	0.40103800
H	-1.49484100	-1.78595400	4.08114700
H	-1.03760000	-3.32304600	4.86474500
H	-2.74469500	-3.00262000	4.46311800
H	-2.45713200	5.03662000	-0.71979000
H	-2.36580000	5.16606200	1.03941800
C	-0.62516000	4.31130900	0.12378700
H	-3.30608000	1.54652100	-3.39281200
H	-3.51025200	3.20792200	-4.00121000
H	-4.82131600	2.43702800	-3.06825700
C	1.39004300	-4.01417000	1.53309900
C	1.11075900	-3.82756400	-0.84493900
C	0.01026000	4.09602200	-1.10227100
C	0.15775300	4.29079100	1.28897600
H	0.98351100	-4.30932500	2.49147900
C	2.65203000	-3.42006900	1.44512300
C	2.37769300	-3.24602700	-0.93578000
O	0.29356000	-4.03217900	-1.94162600
H	-0.60377400	4.09661600	-1.99425200
C	1.38381000	3.84951600	-1.18137700
C	1.53089300	4.04327800	1.21047500
O	-0.50597400	4.52283500	2.47718500
C	3.16282600	-3.02357800	0.19851500

O	3.45810700	-3.18321600	2.53874600
H	2.77096300	-2.91990200	-1.89086800
C	0.88597700	-3.95918000	-3.23178700
C	2.16371400	3.80975300	-0.01367400
O	2.05012000	3.63319000	-2.36714800
H	2.13845200	3.99833400	2.10537300
C	0.26228600	4.59675600	3.66363200
C	4.50699300	-2.32101300	0.07927400
C	3.02024000	-3.64503700	3.80291400
H	1.18572200	-2.93602600	-3.48878700
H	0.11976300	-4.28841900	-3.93579700
H	1.76043300	-4.61742000	-3.30637900
C	3.65033100	3.49028000	-0.06976600
C	1.31466600	3.73983300	-3.57470500
H	0.76401600	3.64563600	3.88632700
H	-0.44023700	4.82769200	4.46702000
H	1.01936800	5.39009600	3.61012500
H	5.00953500	-2.66098300	-0.82931200
H	5.13269800	-2.59592200	0.93126800
C	4.35912000	-0.80806700	0.03229500
H	2.09007700	-3.15350600	4.11799800
H	3.81413400	-3.39479500	4.50931900
H	2.86414200	-4.73178000	3.80847400
H	4.14869300	3.97724800	0.77255900
H	4.07079900	3.90305400	-0.99042900
C	3.93695500	1.99650800	-0.02500900
H	0.53198500	2.97461600	-3.64125600
H	2.03467700	3.58641500	-4.38092900
H	0.85924800	4.73274700	-3.68440200
C	4.26177800	-0.12397800	-1.18965700

C	4.26630500	-0.06735800	1.21445100
C	4.05862000	1.31450300	1.19699000
C	4.05525500	1.25889800	-1.20656400
O	4.37442600	-0.89056100	-2.32966900
H	4.33416900	-0.60678000	2.15152300
O	3.96069300	2.08394500	2.33707700
H	3.95106200	1.79166000	-2.14319800
C	4.32243000	-0.23326600	-3.58392900
C	4.12165200	1.44245300	3.58817300
H	3.35273700	0.25339500	-3.74707500
H	4.46586400	-1.00955300	-4.33805500
H	5.11997000	0.51470200	-3.68329900
H	3.34411700	0.68710000	3.76320900
H	4.03733300	2.22545800	4.34449400
H	5.10546800	0.96298700	3.67737900
C	-0.91042800	-0.72224000	-2.24832900
H	-1.70587400	-0.24648800	-1.68022300
H	-0.71640800	-1.73737600	-1.91200200
Cl	0.57966500	0.23974700	-2.05920100
Cl	-1.45520400	-0.82011000	-3.97108000
H	-5.63063000	-0.76120000	-0.04202100
H	-5.43227300	-0.67040100	1.71089400

Ethyl acetateCDMP[5]A:

C	-2.39020600	3.27787500	-1.23867300
C	-3.38310000	2.29327500	-1.26422500
H	-3.67169300	1.82185500	-2.19510800
C	-4.00955200	1.85257900	-0.09347400
C	-5.03827500	0.73189000	-0.14165100
H	-5.62158800	0.82310800	-1.06110900
H	-5.72408800	0.83845700	0.70199400
C	-4.39712200	-0.64716900	-0.09287400
C	-4.01156700	-1.30706400	-1.27167200
C	-3.36363300	-2.54470000	-1.20279500
H	-3.03722200	-3.04627300	-2.10466900
C	-3.07520100	-3.15473500	0.02166000
C	-3.48043900	-2.50416200	1.19926600
C	-4.13313600	-1.26918500	1.13195400
H	-4.42635500	-0.74607500	2.03412900
C	-2.30619800	-4.46726800	0.06951700
H	-2.63710500	-5.04689500	0.93494900
H	-2.53670900	-5.04607800	-0.82839300
C	-0.80089300	-4.26271000	0.15956400
C	-0.01761900	-4.10236500	-0.99758200
C	1.35395200	-3.84988900	-0.88824000
H	1.95996300	-3.69960000	-1.77412500
C	1.98753100	-3.76961300	0.35690400
C	1.20865400	-3.96058300	1.50967900
C	-0.16469900	-4.19866500	1.40163000
H	-0.77863400	-4.31529100	2.28583900
C	3.47612700	-3.46660200	0.45008300
H	3.98200000	-3.89877500	-0.41580900
C	-2.04188200	3.11410400	-3.60628700
H	-1.79402300	2.04555700	-3.60006200

H	-1.42595100	3.62277000	-4.35063000
H	-3.09860600	3.23972200	-3.87556200
C	-3.79423100	-1.22231000	-3.65894600
H	-2.69979900	-1.25991900	-3.64243700
H	-4.12280900	-0.55176500	-4.45544700
H	-4.20192700	-2.22347100	-3.85089500
C	-3.63663800	-2.55690800	3.58937400
H	-3.16763800	-1.57868300	3.76064900
H	-3.34411100	-3.23909900	4.39016500
H	-4.72734100	-2.43211400	3.60559000
C	0.05405300	-4.06434000	-3.39841000
H	0.43646000	-3.04338200	-3.50913600
H	-0.65004400	-4.26537300	-4.20781600
H	0.88450500	-4.77929800	-3.46096400
C	1.14727300	-4.20000700	3.89469100
H	0.34235400	-3.47593000	4.07823600
H	1.86539600	-4.15241600	4.71569700
H	0.71287500	-5.20730900	3.85467500
O	-1.73997800	3.73160100	-2.36340700
O	-4.30936700	-0.67068200	-2.45267100
O	-3.19312700	-3.15061700	2.38372600
O	-0.68185700	-4.21903500	-2.19556900
O	1.87381600	-3.89545800	2.71797900
C	-3.63175300	2.44382200	1.12285500
C	-2.64986600	3.43901000	1.14717100
H	-2.33823000	3.88652400	2.08238800
C	-2.00794300	3.86411700	-0.01984700
C	-0.90273700	4.90910500	0.03821900
H	-1.09792000	5.58312400	0.87647600
H	-0.92268800	5.50321400	-0.87886900
C	0.48244800	4.30100000	0.20045500
C	0.99922700	3.99841700	1.47213900

C	2.24752000	3.38401000	1.59800900
H	2.63933400	3.12054000	2.57153500
C	3.02367400	3.05993000	0.47968400
C	2.52356900	3.39558700	-0.78815400
C	1.26969200	4.00174300	-0.91435800
H	0.86432700	4.22996300	-1.89250200
C	4.35658500	2.34347600	0.64748400
H	5.03244600	2.65165300	-0.15411800
H	4.80354800	2.64827000	1.59801000
C	4.21588300	0.82878200	0.61940700
C	3.83665300	0.11012900	1.76860300
C	3.61732500	-1.26615400	1.70046500
H	3.29964300	-1.82265700	2.57325100
C	3.77960600	-1.97685600	0.50348600
C	4.20463400	-1.26910300	-0.62819500
C	4.41453600	0.11262000	-0.56056000
H	4.70513100	0.66423600	-1.44730100
H	3.87865200	-3.94504500	1.34710800
C	-3.98804000	2.61411400	3.48654900
H	-2.93753500	2.48268600	3.77859800
H	-4.62861200	2.13518200	4.22979400
H	-4.21362400	3.68825500	3.45716700
C	0.72583800	4.12126700	3.84886200
H	0.89551800	3.05366600	4.04157000
H	-0.02936100	4.49531400	4.54293000
H	1.66594300	4.66357600	4.01472400
C	3.05153600	3.75641500	-3.09704600
H	2.12342700	3.39949200	-3.56139900
H	3.88777300	3.52734400	-3.76090000
H	2.98347700	4.84265200	-2.95799500
C	3.37284600	0.15132800	4.11790900
H	2.38985400	-0.33208700	4.04747000

H	3.34811400	0.90338100	4.90903200
H	4.12354400	-0.60908600	4.36955600
C	5.38495400	-1.54459400	-2.69387200
H	5.08712600	-0.64650300	-3.24945200
H	5.54389300	-2.35764100	-3.40586600
H	6.32009400	-1.33680100	-2.15981900
O	-4.27572000	1.98302500	2.25290500
O	0.21233900	4.34625100	2.54908800
O	3.32526400	3.09338900	-1.87225200
O	3.70523400	0.84272700	2.92752400
O	4.37010000	-1.98688200	-1.80193100
C	2.01217700	0.02724900	-3.53135600
H	1.88689200	0.12014100	-4.61041900
H	2.61488600	-0.85788200	-3.30307000
H	2.53674700	0.89067700	-3.11650500
C	0.66268100	-0.12995700	-2.87218900
O	-0.36780300	-0.40296900	-3.46712200
O	0.75454900	0.03766600	-1.55066400
C	-0.10340200	0.04995000	0.68495800
H	0.65426200	-0.66731500	1.01105400
H	-1.00342400	-0.08851700	1.29134700
H	0.27606800	1.06165000	0.84859400
C	-0.45696200	-0.16508900	-0.77157200
H	-0.82329500	-1.17639900	-0.95917400
H	-1.21478600	0.54195200	-1.11539600

AcetoneCDMP[5]A:

C	1.05210500	4.85151400	-0.00604600
C	2.11884600	3.76652800	-0.00136200
C	-0.35910500	4.29805500	0.11880700
C	2.71181200	3.35436100	1.19581900
C	2.51709400	3.13507300	-1.19204500
C	-1.11397400	3.99954000	-1.01912400
C	-0.93393100	4.04674200	1.37641200
H	2.38869000	3.83841900	2.10874900
C	3.66398900	2.33137400	1.22694700
C	3.47719100	2.11959300	-1.16142400
O	1.91428900	3.57607300	-2.34853100
H	-0.66298400	4.18861300	-1.98552300
C	-2.39526900	3.44642800	-0.92541100
C	-2.21108000	3.48877100	1.46947400
O	-0.17158700	4.38396000	2.47303200
C	4.05851400	1.69703500	0.03819800
O	4.25989500	1.88227400	2.38801300
H	3.77376500	1.60961900	-2.06917900
C	2.31880400	2.98862900	-3.57786500
C	-2.95756300	3.16904000	0.33059000
O	-3.16343700	3.13136100	-2.03031200
H	-2.64922600	3.26568200	2.43348200
C	-0.73726000	4.20556100	3.75845600
C	5.05169900	0.54416100	0.04879000
C	3.95892400	2.55821100	3.59400400
H	3.39081600	3.13762200	-3.76101300
H	1.75101800	3.50262600	-4.35606400
H	2.09107800	1.91684700	-3.61212300

C	-4.32465500	2.51266900	0.46202100
C	-2.79698400	3.70477000	-3.27623100
H	-1.65896300	4.78909600	3.88231100
H	0.00921500	4.56205000	4.47086200
H	-0.95694100	3.14969900	3.96453000
H	5.68342800	0.60717500	-0.84053800
H	5.69653800	0.63283600	0.92587500
C	4.35486800	-0.80708200	0.07250200
H	4.22090800	3.62321400	3.54062300
H	4.56164200	2.08073500	4.36919800
H	2.89671500	2.47014500	3.85909800
H	-4.79094600	2.85035100	1.39150300
H	-4.95914200	2.83448100	-0.36761100
C	-4.24258400	0.99368200	0.46217000
H	-2.68424900	4.79327300	-3.19874400
H	-3.60907600	3.47275100	-3.96809900
H	-1.86519100	3.27767200	-3.66811000
C	3.99252200	-1.39907300	1.28582800
C	4.01025900	-1.46464000	-1.12077000
C	-4.39566700	0.26952400	-0.72158100
C	-3.95908500	0.27982600	1.64048100
H	4.25509400	-0.87634900	2.19772700
C	3.28410200	-2.60300600	1.32805100
C	3.29374500	-2.66531700	-1.07672800
O	4.41957000	-0.86333900	-2.28663600
H	-4.60874900	0.82182300	-1.62904900
C	-4.23663300	-1.12007600	-0.75819600
C	-3.79346300	-1.10557700	1.60316700
O	-3.85977100	1.02540500	2.79434600
C	2.91223900	-3.24658000	0.13629900

O	2.90615700	-3.22302700	2.50198000
H	2.99259600	-3.16099800	-1.99092200
C	4.01535100	-1.44520300	-3.52056600
C	-3.91244600	-1.82670500	0.40891600
O	-4.35004600	-1.85746900	-1.92277900
H	-3.54596300	-1.66023300	2.49934600
C	-3.63669700	0.33952800	4.01339600
C	2.08732900	-4.52475000	0.15667800
C	3.33085900	-2.64774400	3.72333900
H	4.40055400	-2.46764000	-3.62855900
H	4.45478300	-0.81984200	-4.30023300
H	2.92525700	-1.43771900	-3.62235700
C	-3.66450400	-3.32755100	0.38870700
C	-5.11719900	-1.30381400	-2.98210400
H	-4.43693900	-0.38103200	4.22652900
H	-3.62700200	1.10317400	4.79356300
H	-2.67496200	-0.18969800	4.01410900
H	2.31862700	-5.11070300	-0.73613000
H	2.36900900	-5.12000300	1.02927400
C	0.58995800	-4.26061400	0.20614400
H	4.42505000	-2.57972700	3.78307800
H	2.97125400	-3.31049600	4.51317100
H	2.90704800	-1.64592500	3.87392500
H	-4.10085200	-3.77272000	1.28673100
H	-4.16933100	-3.75878900	-0.47836800
C	-2.18554600	-3.68032300	0.33125500
H	-6.09147200	-0.94794900	-2.62502900
H	-5.26639200	-2.10959300	-3.70378100
H	-4.59714600	-0.47616900	-3.48043400
C	-0.16189000	-4.10099800	-0.97111600

C	-0.07025700	-4.14612200	1.43178300
C	-1.43642100	-3.86174600	1.50465900
C	-1.52898800	-3.81184300	-0.89804500
O	0.52480800	-4.25614700	-2.15223600
H	0.52159300	-4.25942700	2.33098600
O	-2.12331300	-3.74132900	2.69604400
H	-2.11417600	-3.67670000	-1.80020400
C	-0.19129500	-4.15254600	-3.37081300
C	-1.42814600	-4.02658000	3.89651500
H	-1.00994500	-4.88197300	-3.42417900
H	0.52925900	-4.36436900	-4.16252300
H	-0.59531300	-3.14423200	-3.52214600
H	-1.02484300	-5.04749500	3.89994700
H	-2.15938100	-3.92836600	4.70128700
H	-0.60452600	-3.32142600	4.06999300
C	-0.12536500	-0.18152800	-2.79693900
C	-1.57479300	-0.03590600	-3.21711600
C	0.16643700	-0.08454300	-1.31766000
O	0.74941400	-0.36879800	-3.63141900
H	-2.03236000	0.84548300	-2.75603700
H	-2.14627300	-0.90118300	-2.86078700
H	-1.63934300	0.02238300	-4.30552300
H	1.20159000	-0.35663500	-1.11237800
H	-0.51258800	-0.72847700	-0.74892700
H	-0.01234900	0.94401100	-0.98108900
H	1.12647100	5.42214000	-0.93529700
H	1.24169300	5.53776100	0.82344900

5. References

- [S1] L. Pauling, The nature of the chemical bond, Cornell University Press, Ithaca, NY, 1939.