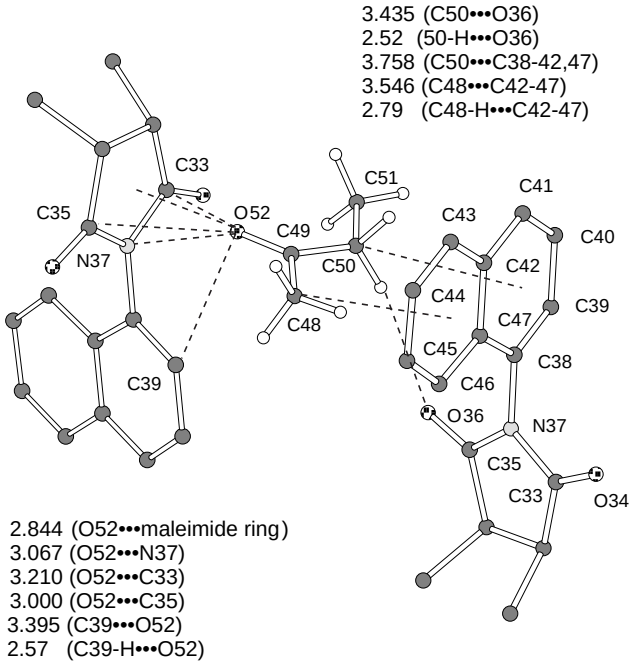
Electronic Supporting Information

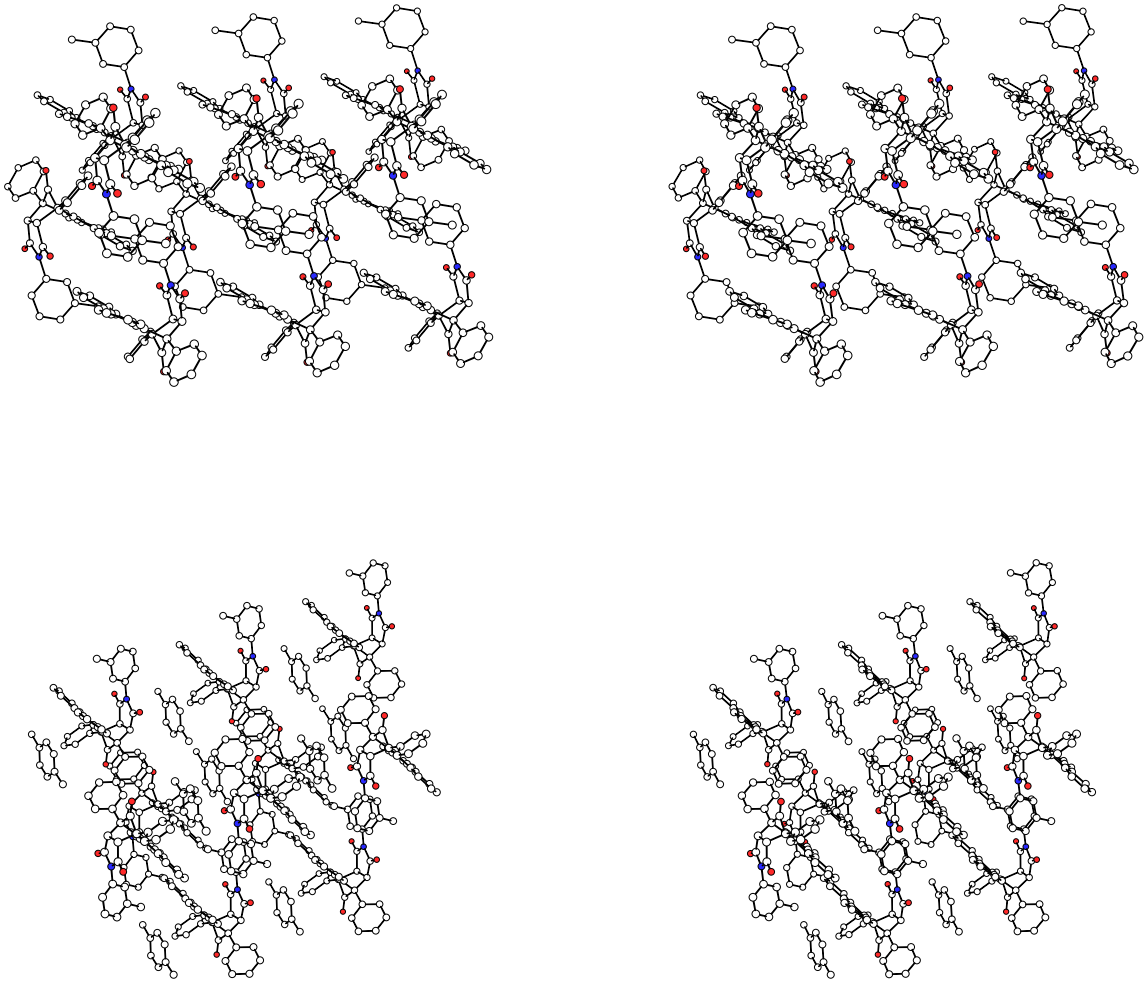
Non-hydroxylic Clathrate Hosts of [4+2]π Cycloadducts of Phencyclone and *N*-Arylmaleimides. Recognition of Aromatic Guests

Yasuyuki Yoshitake,[a] Junichi Misaka,[a] Koji Setoguchi,[a] Masaki Abe,[a] Tomohiro Kawaji,[a] Masashi Eto[b] and Kazunobu Harano[a]*

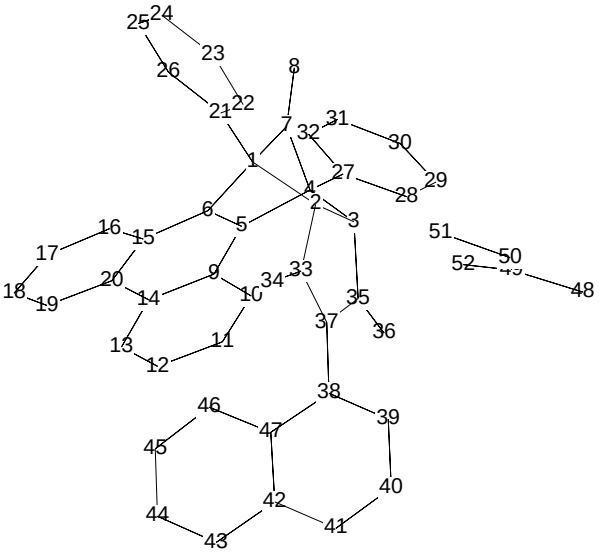
[a]*Faculty of Pharmaceutical Sciences, Kumamoto University, 5-1 Oe-hon-machi, Kumamoto 862-0973, Japan.School of Agriculture,* [b]*Kyushu Tokai University, 5435 Kawayo, Choyo-son, Asogun, Kumamoto 869-1404, Japan*
(E-mail: harano@gpo.kumamoto-u.ac.jp)



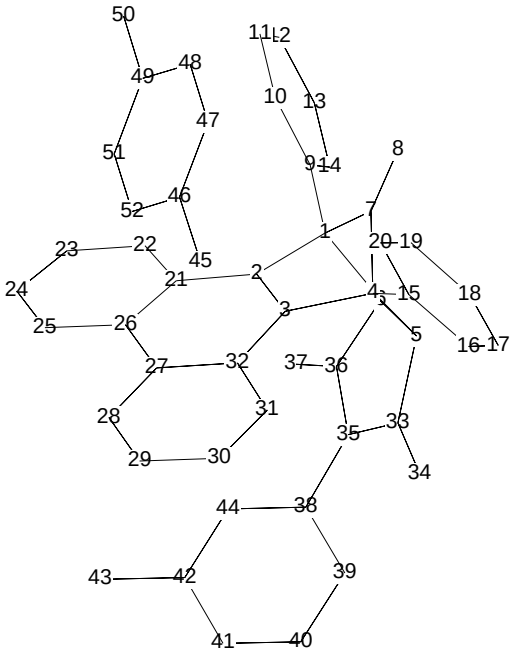
ESI-1. Intermolecular atom-plane and atom-atom distances (Å) of the **3c**•butanone complex



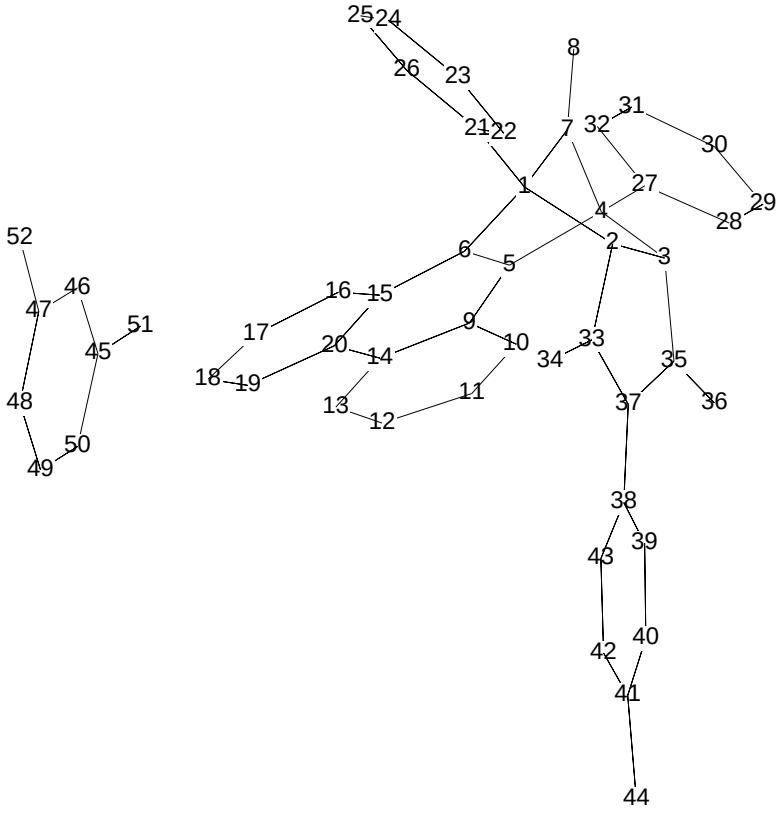
ESI-2. Stereo drawings of the crystal structure of the free host (**3g**) and the inclusion complex of **3g**•*p*-xylene.



ESI-3. Numering sequence of **3c•**butanone

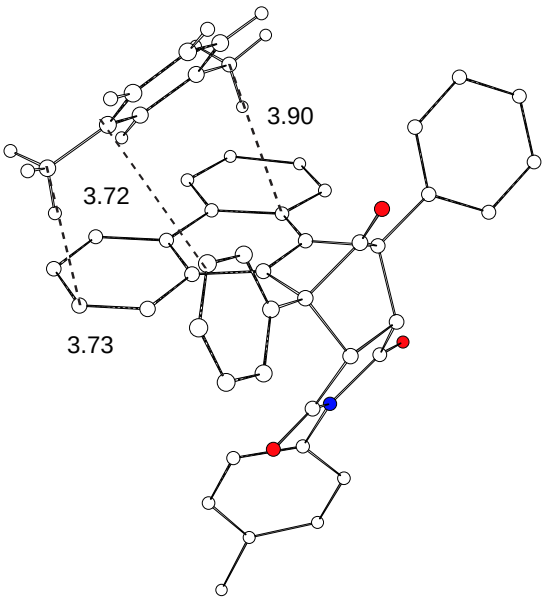


ESI-4. Numering sequence of of the free host (**3g**) and the inclusion complex of **3g**•*p*-xylene

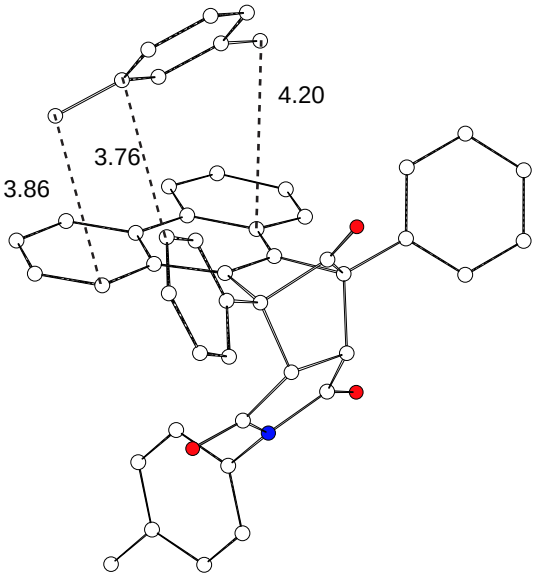


ESI-5. Numering sequence of **2h**•*m*-xylene

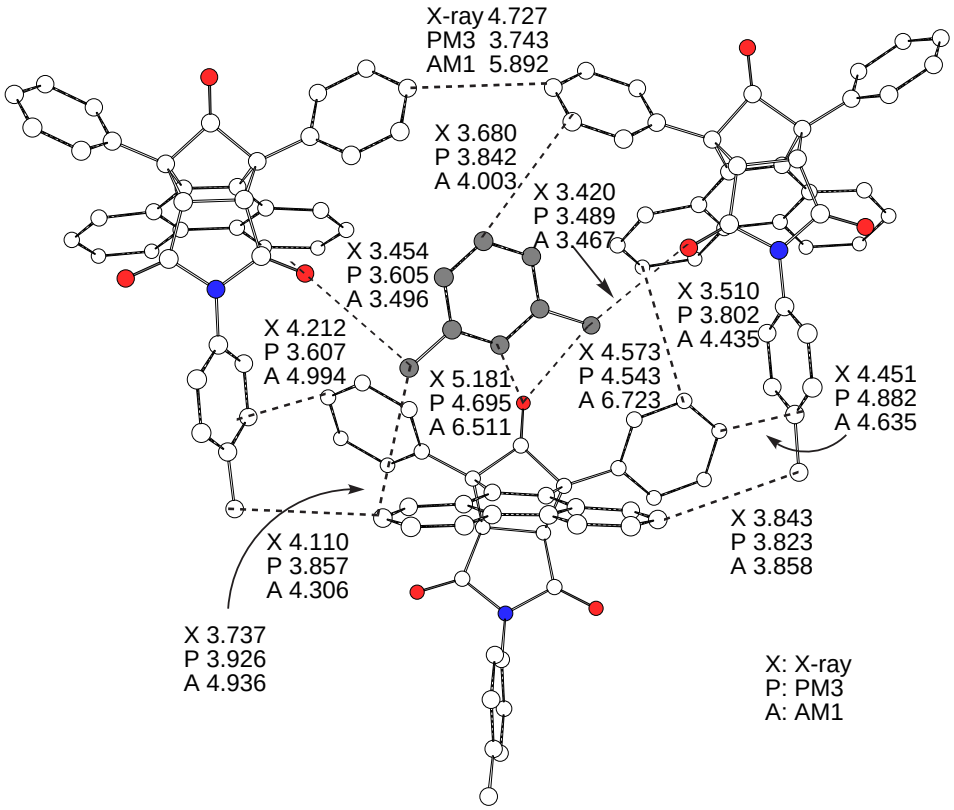
X-Ray



PM3



ESI-6. X-Ray and PM3 stuctures of the 1:1 complex model of m-xylene and **3h**



ESI-7. PM3-Calculated Geometry of 3:1 Complex extracted from the inclusion compound **3h** ÅE*m* -xylene and Comparison of the Interatomic Distance Data between the PM3- and AM1-Calculated Data and X-Ray Data

ESI-8. Heats of formation[a] for the complex formation of **3h**•*m*-xylene calculated by PM3 method

compound	ΔHf^{b}	$\Delta\Delta Hf^{b}$
m-xylene	4.786 (6.851)	
3h	60.082 (100.221)	
3h (1 mol) + *m*-xylene	64.868 (107.072)	0.0
3h (1 mol) •*m*-xylene	61.232 (106.999)	-3.636 (-0.073)

a) In kcal/mol. b) AM1 values in parentheses.