Electronic Supplementary Material for CrystEngComm

A robust conglomerate structure type in salts of cationic organopalladium complexes and non-coordinating anions

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Lattice energy minimizations for ***rac*-2e** *vs.* ***R*-2e** and ***rac*-3** *vs.* ***R*-3**.

a) **Van-der-Waals interactions** were modeled with a Buckingham potential of the type

$$E_{vdW} = \frac{1}{2}\sum_i \sum_j (-Ar_{ij}^{-6} + Be^{-Cr_{ij}})$$

Van-der-Waals parameters in lattice energy minimizations for ***rac*-2e** *vs.* ***R*-2e** and ***rac*-3** *vs.* ***R*-3**.

atom type 1	atom type 2	A_{ij}	B_{ij}	C_{ij}
		[kJ·mol^{-1}·Å^{-6}]	[kJ·mol^{-1}]	[Å^{-1}]
H	H	144.2	11104	3.74
H	C	523	36677	3.67
C	C	2377	349908	3.60
N	N.	1800	361000	3.90
O	O	1242.6	372203	4.18
F	F	858.2	425692	4.50
P	P	6840.2	466827	3.29
S	S	6840.2	466827	3.29
Pd	Pd	6463	1804000	4.00

For all other mixed interactions the combining rules were used:

$A_{12} = \sqrt{A_{11} \cdot A_{22}}$

$B_{12} = \sqrt{B_{11} \cdot B_{22}}$

$C_{12} = \frac{(C_{11} + C_{22})}{2}$

b) **Hydrogen bond interactions** were modeled by additional exponential functions.

N-H···O $E = -8184.5 \cdot \exp(-2.9 \cdot r_{ij})$

N-H···F $E = -9100 \cdot \exp(-3.18 \cdot r_{ij})$

with E in kJ·mol^{-1} and hydrogen-acceptor distances r_{ij} in Å.

c) Results of lattice energy minimizations for ***rac*-2e** *vs.* ***R*-2e**

	***rac*-2e**		***R*-2e**	
	experimental	minimized	experimental	minimized
space group	$P2_1/c$	$P2_1/c$	$P2_1$	$P2_1$
T (K) experiment [a]	293		130	
a (Å)	7.724(3)	7.888	7.5980(5)	7.575
b (Å)	20.015(8)	18.874	20.5971(14)	20.546
c (Å)	14.106(6)	13.649	13.8222(9)	13.707
β (°)	102.012(9)	104.95	105.038(2)	104.63
V (Å^3)	2133.0(15)	1963.2	2089.1(2)	2064.2
E total (kJ·mol^{-1}) [b]		-183.4		-166.1
E H bonds (kJ·mol^{-1}) [c]		-34.3		-24.4

d) Results of lattice energy minimizations for ***rac*-3** *vs.* ***R*-3**.

	***rac*-3**		***R*-3**	
	experimental	minimized	experimental	minimized
space group	$P2_1/n$		$P2_1$	
T (K) experiment [a]	110		130	
a (Å)	11.6744(17)	12.199	11.6452(13)	11.782
b (Å)	14.108(2)	13.636	14.3172(13)	14.291
c (Å)	11.9538(18)	11.965	12.0277(13)	11.791
β (°)	96.137(4)	102.51	96.018(4)	98.04
V (Å^3)	1957.5(5)	1943.0	1994.3(4)	1965.8
E total (kJ·mol^{-1}) [b]		-167.4		-148.3
E H bonds (kJ·mol^{-1}) [c]		-18.6		-20.0

[a] The unit cell volumes after minimization are usually lower than the experimental values because the latter refer to finite temperatures >> 0 K. The difference is therefore most marked for ***rac*-2e**.

[b] Lattice energy/ion pair, taking into account both van der Waals interactions and H bonds.

[c] Hydrogen bond energy/ion pair.