Supporting Information

Sublimation thermodynamic aspects of adamantane and memantine derivatives of sulfonamide molecular crystals

German L. Perlovich[*]*, Tatiana V. Volkova*

G.A. Krestov Institute of Solution Chemistry, Russian Academy of Sciences, 153045 Ivanovo, Russia;

[*] To whom correspondence should be addressed:

Telephone: +7-4932-533784; Fax: +7-4932-336237; E-mail glp@isc-ras.ru

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Table 1S
Source, purification, and analysis details of the studied samples

№	Chemical name	M/g mole^{-1}	Sourse	Method Purification	Final mole fraction purity	Analysis method
5	N-Adamantan-1-yl-4-bromo-benzenesulfonamide	370.3	synthesis	recrystallization	0.99	HPLC
6	N-(3,5-Dimethyl-adamantan-1-yl)-4-bromo-benzenesulfonamide	398.36	synthesis	recrystallization	0.99	HPLC
7	N-Adamantan-1-yl-4-trifluoromethyl-benzenesulfonamide	312.4	synthesis	recrystallization	0.99	HPLC
8	N-(3,5-Dimethyl-adamantan-1-yl)-4-trifluoromethyl-benzenesulfonamide	340.48	synthesis	recrystallization	0.99	HPLC
9	N-Adamantan-1-yl-4-nitro-benzenesulfonamide	336.41	synthesis	recrystallization	0.99	HPLC
10	N-(3,5-Dimethyl-adamantan-1-yl)-4-nitro-benzenesulfonamide	364.47	synthesis	recrystallization	0.99	HPLC
	Ethanol	46.07	Sigma-Aldrich	none	≥0.99	

Table 2S
Temperature dependencies of saturation vapor pressure of studied compounds

2[a]		**5**[b]		**6**[c]		**7**[d]		**8**[e]		**9**[f]		**10**[g]	
t /°C	*P* /Pa	t /°C	*P* /Pa	t /°C	*P* /Pa	t /°C	*P* /Pa	t /°C	*P* /Pa	t /°C	*P* /Pa	t /°C	*P* /Pa
113.0	$2.55\cdot10^{-1}$	125.0	$5.23\cdot10^{-2}$	105.0	$1.40\cdot10^{-2}$	120.0	$3.59\cdot10^{-1}$	73.0	$6.78\cdot10^{-2}$	129.0	$2.13\cdot10^{-2}$	111.0	$7.30\cdot10^{-3}$
114.0	$2.73\cdot10^{-1}$	126.0	$5.53\cdot10^{-2}$	106.0	$1.56\cdot10^{-2}$	122.0	$4.45\cdot10^{-1}$	75.0	$8.65\cdot10^{-2}$	131.0	$2.43\cdot10^{-2}$	112.0	$8.12\cdot10^{-3}$
115.0	$2.92\cdot10^{-1}$	129.0	$7.46\cdot10^{-2}$	108.0	$2.08\cdot10^{-2}$	123.0	$4.83\cdot10^{-1}$	77.0	$1.02\cdot10^{-1}$	132.0	$2.67\cdot10^{-2}$	113.0	$8.97\cdot10^{-3}$
118.0	$4.19\cdot10^{-1}$	132.0	$9.49\cdot10^{-2}$	111.0	$2.93\cdot10^{-2}$	124.0	$5.49\cdot10^{-1}$	79.0	$1.24\cdot10^{-1}$	135.0	$3.54\cdot10^{-2}$	115.0	$1.12\cdot10^{-2}$
120.0	$4.74\cdot10^{-1}$	133.0	$1.00\cdot10^{-1}$	113.0	$3.74\cdot10^{-2}$	126.0	$6.92\cdot10^{-1}$	80.0	$1.46\cdot10^{-1}$	136.0	$3.85\cdot10^{-2}$	117.0	$1.38\cdot10^{-2}$
121.0	$5.55\cdot10^{-1}$	135.0	$1.18\cdot10^{-1}$	115.0	$4.61\cdot10^{-2}$	128.0	$8.14\cdot10^{-1}$	81.0	$1.52\cdot10^{-1}$	139.0	$4.92\cdot10^{-2}$	118.0	$1.49\cdot10^{-2}$
122.0	$5.92\cdot10^{-1}$	138.0	$1.50\cdot10^{-1}$	118.0	$6.17\cdot10^{-2}$	129.0	$9.48\cdot10^{-1}$	83.0	$1.92\cdot10^{-1}$	143.0	$6.70\cdot10^{-2}$	119.0	$1.71\cdot10^{-3}$
123.0	$6.19\cdot10^{-1}$	140.0	$1.75\cdot10^{-1}$	119.0	$7.29\cdot10^{-2}$	130.0	$9.93\cdot10^{-1}$	85.0	$2.24\cdot10^{-1}$	147.0	$9.01\cdot10^{-2}$	121.0	$2.09\cdot10^{-2}$
125.0	$7.64\cdot10^{-1}$	142.0	$2.10\cdot10^{-1}$	120.0	$7.85\cdot10^{-2}$	131.0	1.15	87.0	$2.78\cdot10^{-1}$	149.0	$1.10\cdot10^{-1}$	122.0	$2.35\cdot10^{-2}$
126.0	$8.40\cdot10^{-1}$	144.0	$2.38\cdot10^{-1}$	122.0	$9.72\cdot10^{-2}$	132.0	1.22	89.0	$3.40\cdot10^{-1}$	151.0	$1.25\cdot10^{-1}$	124.0	$2.85\cdot10^{-2}$
128.0	1.03	146.0	$2.78\cdot10^{-1}$	124.0	$1.26\cdot10^{-1}$	133.0	1.36	91.0	$4.05\cdot10^{-1}$	152.0	$1.33\cdot10^{-1}$	125.0	$3.10\cdot10^{-2}$
129.0	1.08	148.0	$3.45\cdot10^{-1}$	126.0	$1.52\cdot10^{-1}$	134.0	1.51	93.0	$4.91\cdot10^{-1}$	155.0	$1.69\cdot10^{-1}$	126.0	$3.54\cdot10^{-2}$
131.0	1.28	150.0	$3.91\cdot10^{-1}$			136.0	1.93	95.0	$5.85\cdot10^{-1}$	157.0	$2.02\cdot10^{-1}$	127.0	$3.70\cdot10^{-2}$
132.0	1.40	152.0	$4.58\cdot10^{-1}$			138.0	2.26			158.0	$2.17\cdot10^{-1}$	128.0	$4.35\cdot10^{-2}$
133.0	1.50	154.0	$5.57\cdot10^{-1}$							162.0	$2.92\cdot10^{-1}$	129.0	$4.94\cdot10^{-2}$
										164.0	$3.25\cdot10^{-1}$		

[a] $\ln(P/\text{Pa}) = (35.3 \pm 0.4) - (14153 \pm 172)/T$; $\sigma = 9.4\cdot10^{-3}$; r = 0.9990; n=15
[b] $\ln(P/\text{Pa}) = (31.5 \pm 0.3) - (13460 \pm 298)/\text{T}$; $\sigma = 8.4\cdot10^{-3}$; r = 0.9995; n = 15
[c] $\ln(P/\text{Pa}) = (40.9 \pm 0.4) - (17076 \pm 160)/\text{T}$; $\sigma = 6.2\cdot10^{-3}$; r = 0.9996; n=12
[d] $\ln(P/\text{Pa}) = (41.1 \pm 0.4) - (16578 \pm 173)/\text{T}$; $\sigma = 5.3\cdot10^{-3}$; r = 0.9994; n = 14
[e] $\ln(\text{P/Pa}) = (33.2 \pm 0.3) - (12433 \pm 104)/\text{T}$; $\sigma = 4.3\cdot10^{-3}$; r = 0.9996; n = 13
[f] $\ln(P/\text{Pa}) = (30.6 \pm 0.2) - (13872 \pm 72)/\text{T}$; $\sigma = 4.7\cdot10^{-3}$; r = 0.9998; n=16
[g] $\ln(P/\text{Pa}) = (37.1 \pm 0.4) - (16135 \pm 147)/\text{T}$; $\sigma = 5.9\cdot10^{-3}$; r = 0.9995; n=15

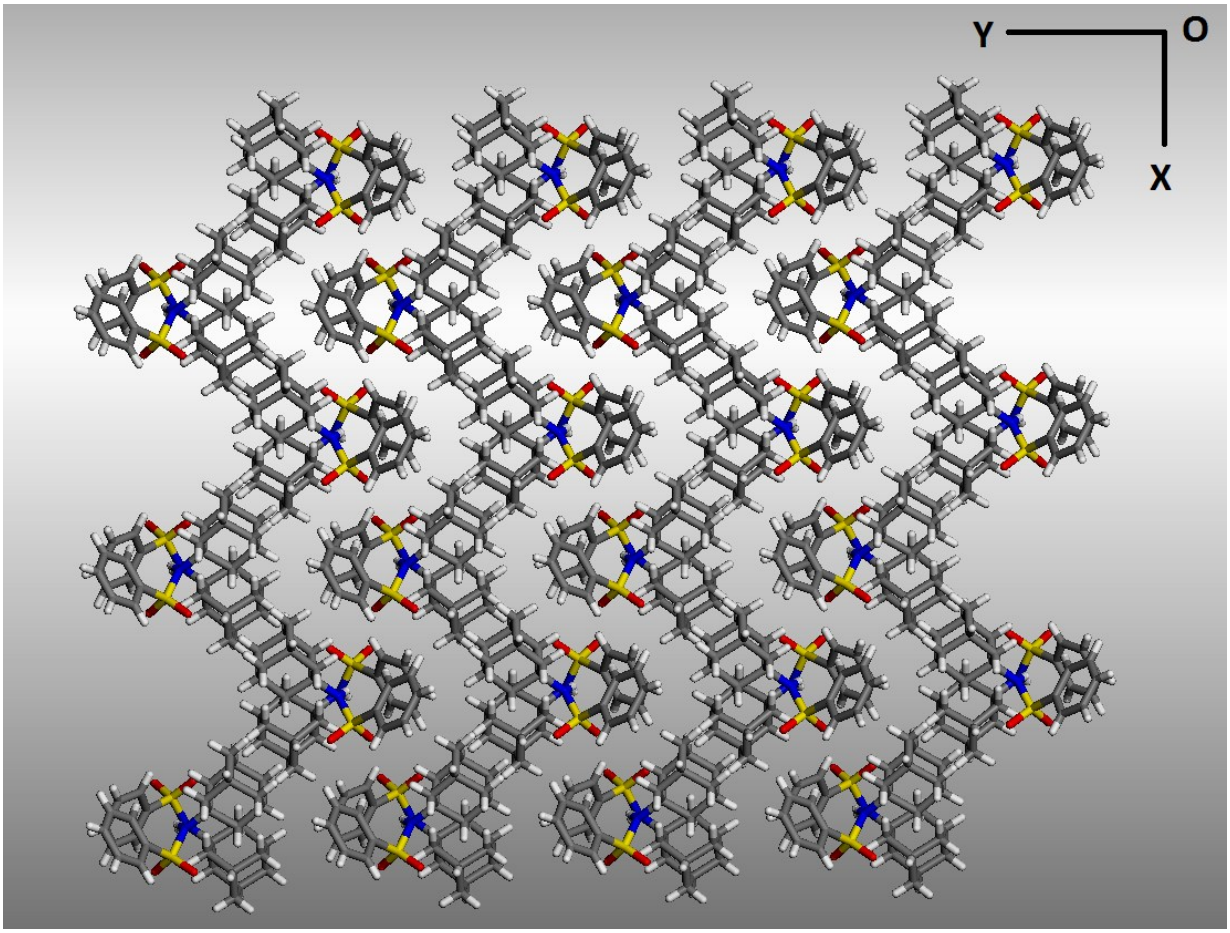
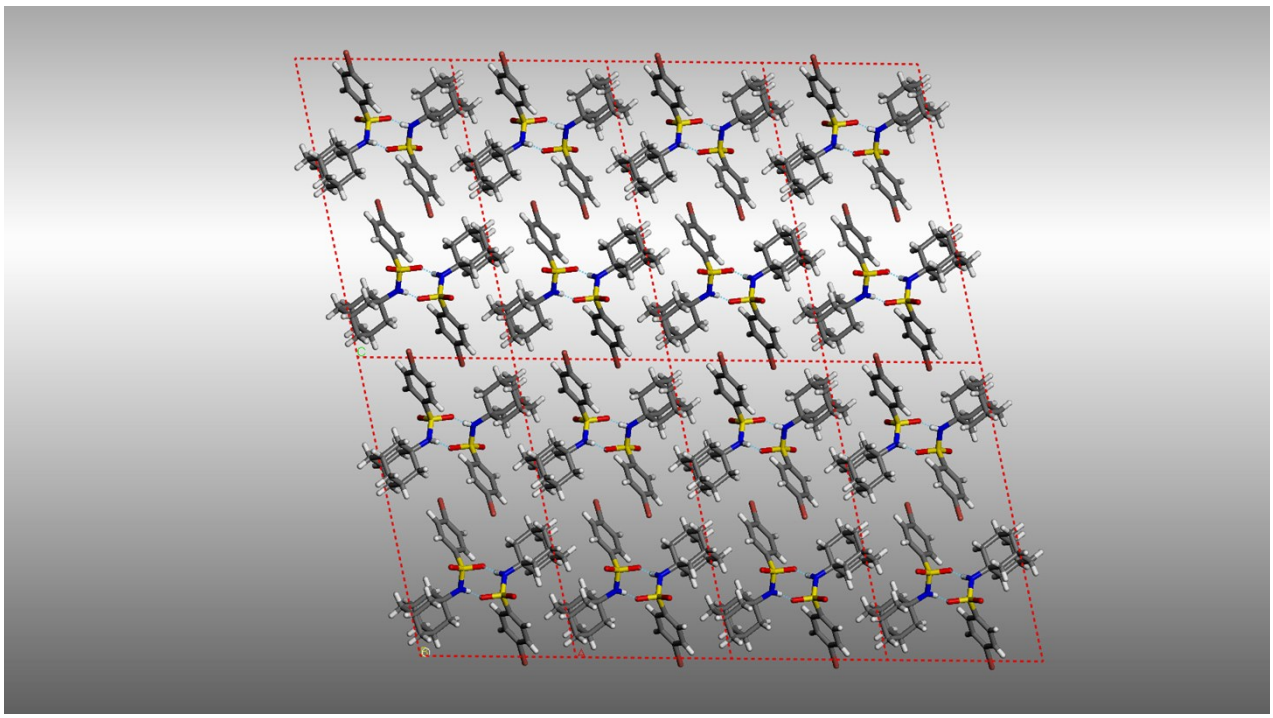
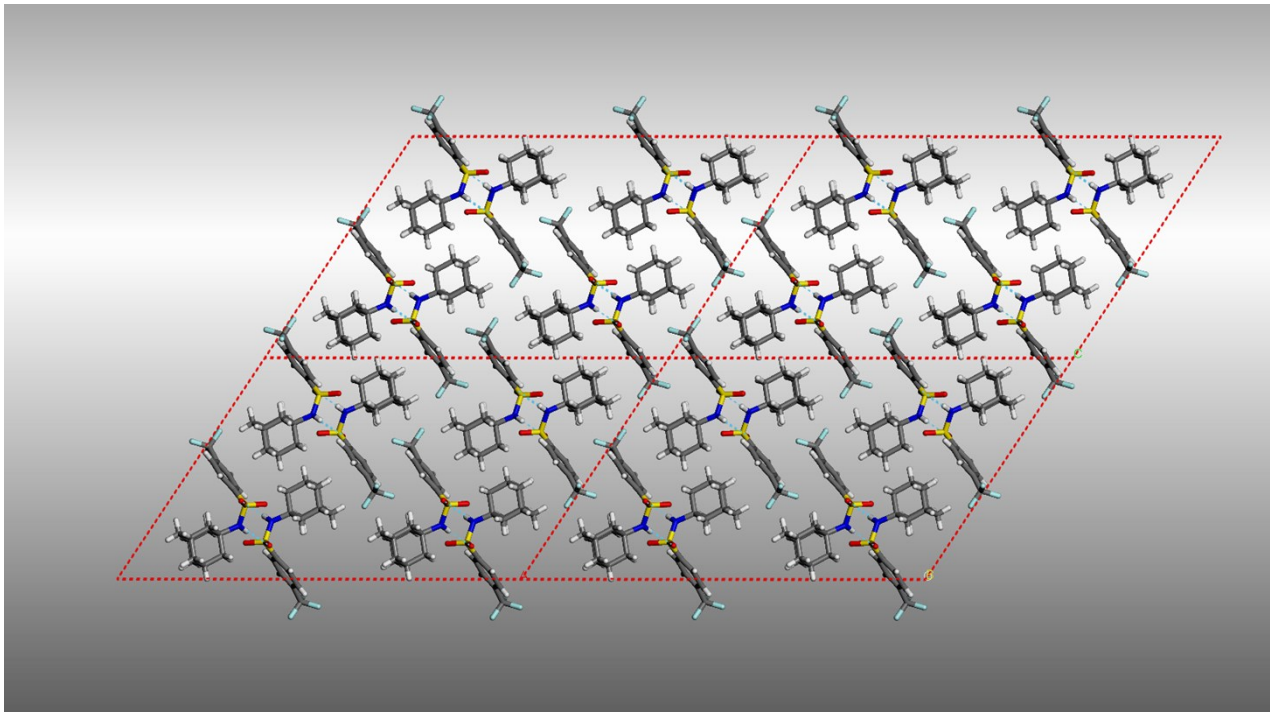


Figure 1S Molecular packing architecture of crystal **1**



a



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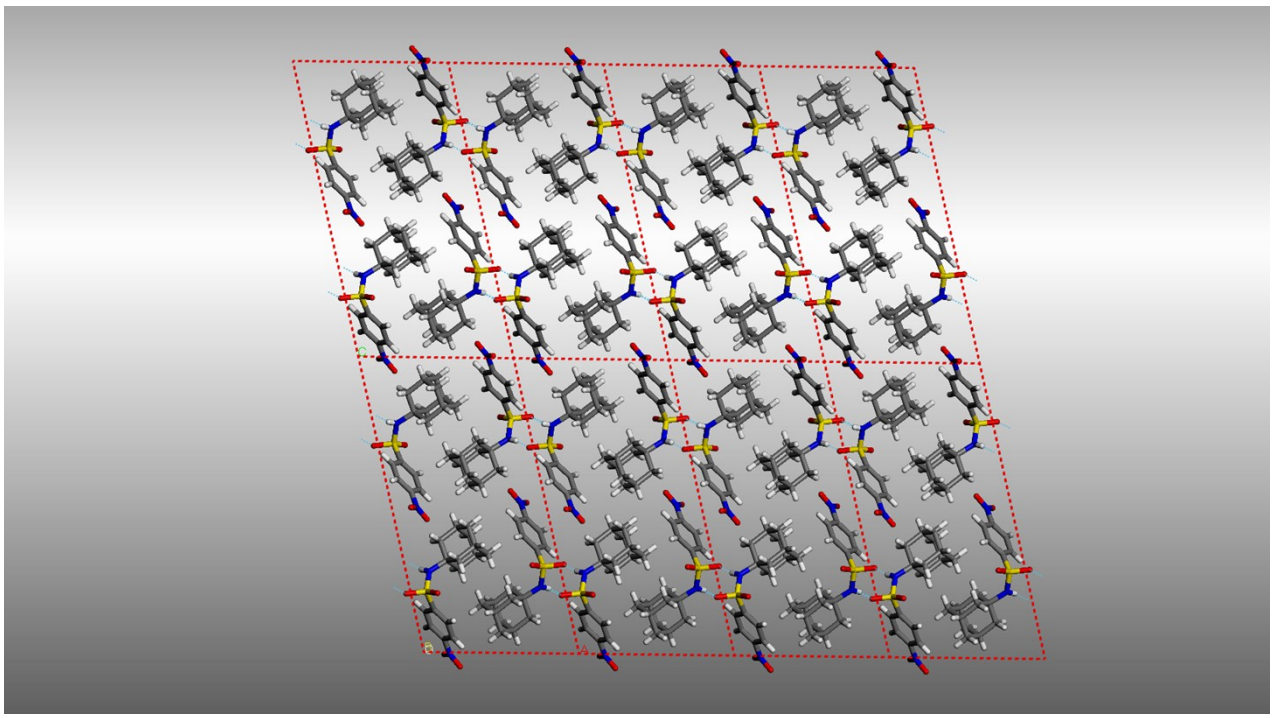
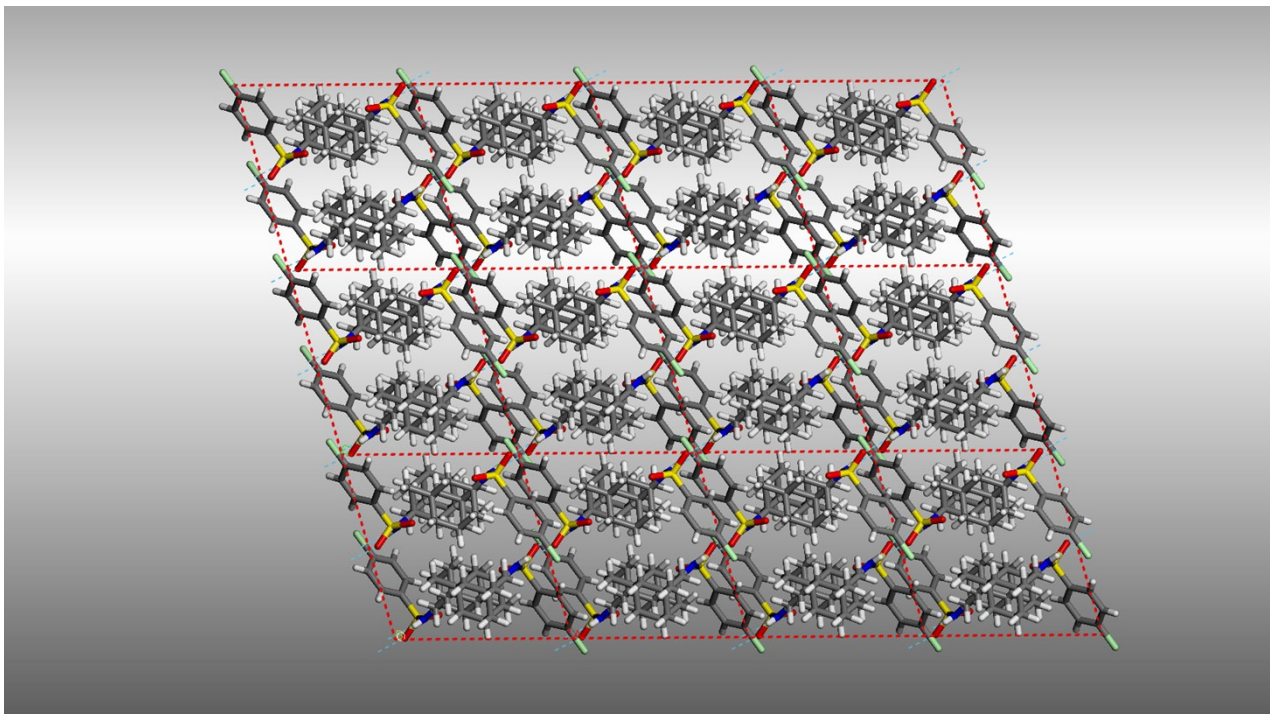
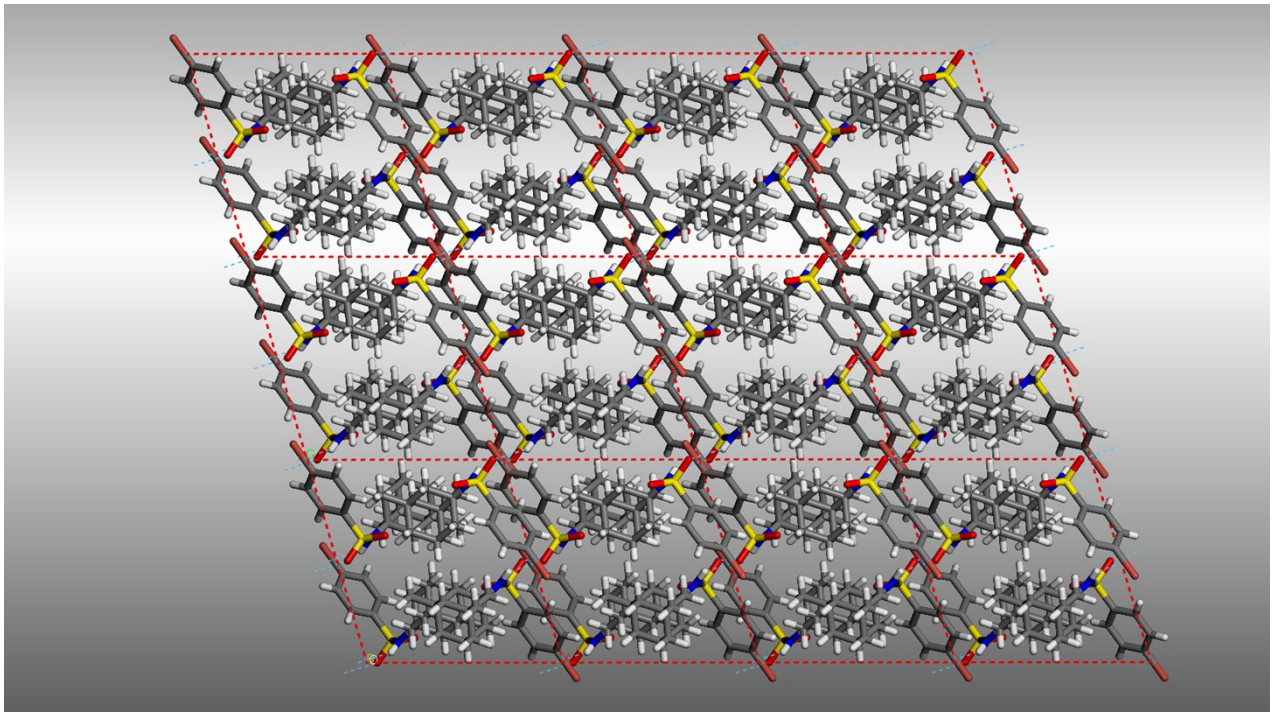


c

Figure 2S. Molecular packing architectures of crystals **5** (a), **7** (b) and **9** (c).



a



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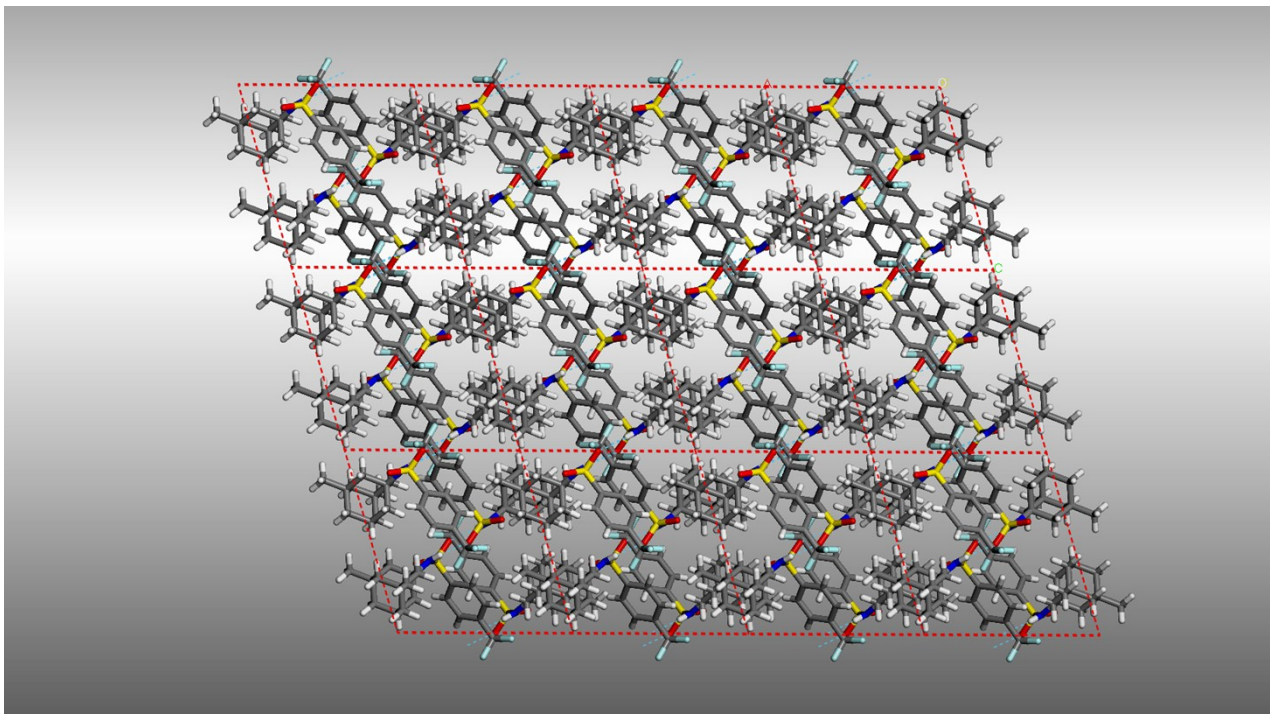

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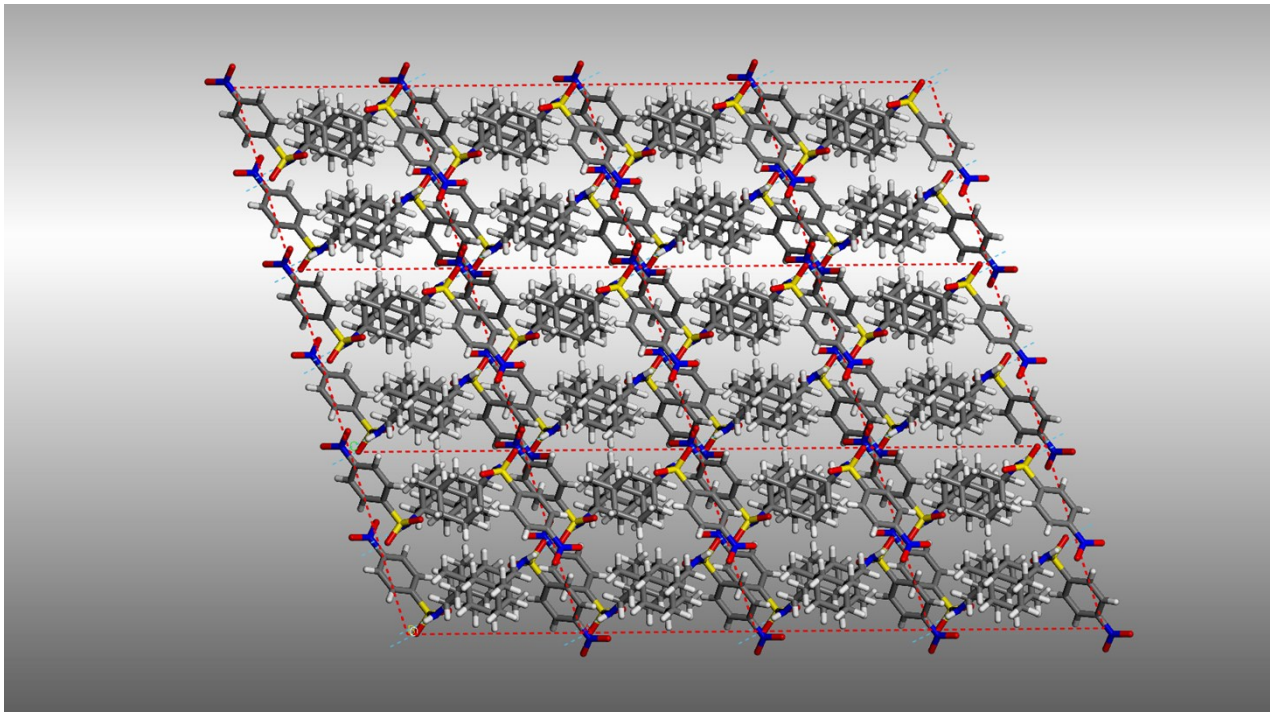

d

Figure 3S. Molecular packing architectures of crystals **4** (a), **6** (b), **8** (c) and **10** (d).

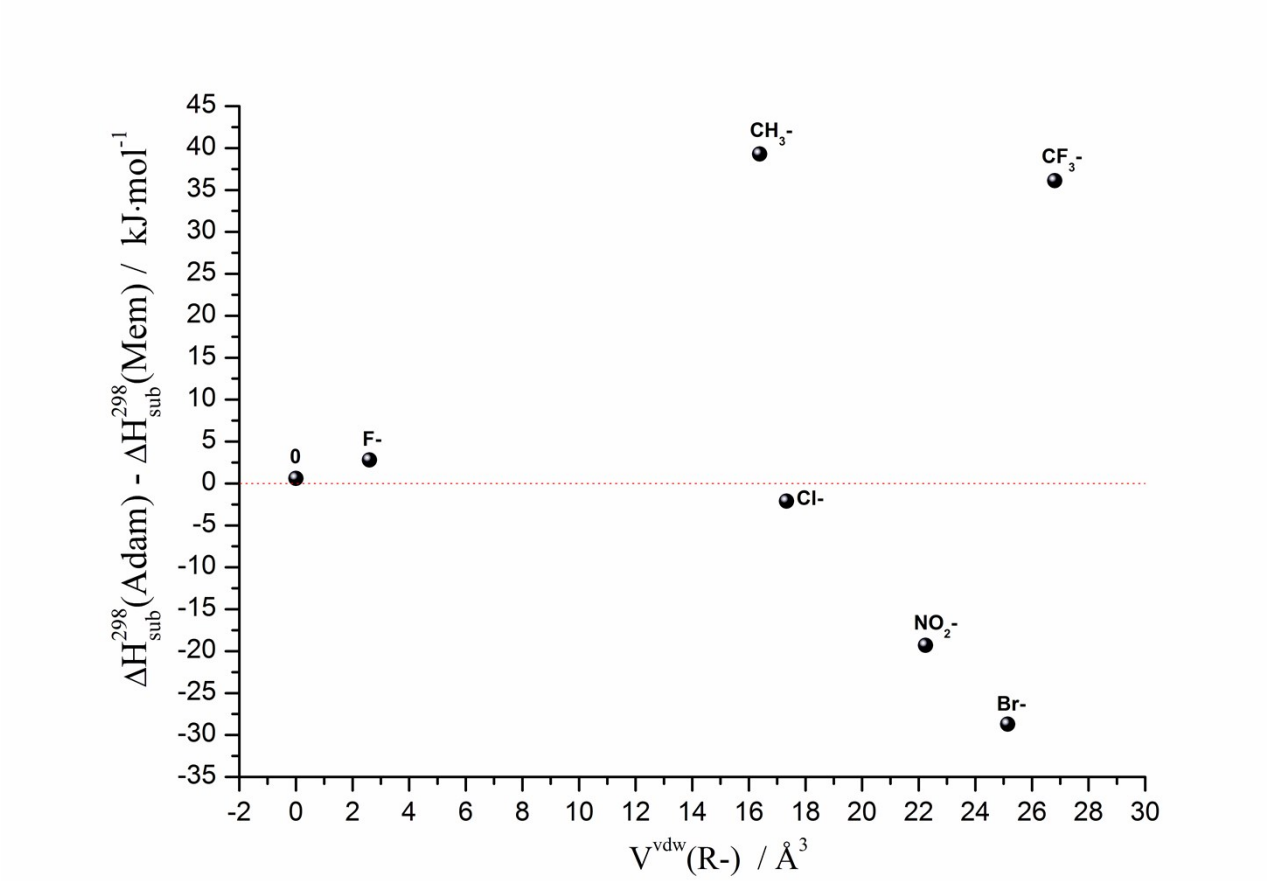

Figure 4S. Experimental data in the coordinates of difference of the sublimation enthalpy terms (OY-coordinate) of the compounds with adamantane fragment to the compounds with memantine fragment versus van-der-Waals volumes of the atom located at para- position of the phenyl ring. Red dotted line corresponds to zero OY-value, **0** – corresponds to the unsubstituted substances.