

## Supporting Information:

### Fine tuning the optical properties and frontier orbital energy in pyrrolylenones as an example of the D- $\pi$ -A sensitizer due to functionalization of molecular backbone

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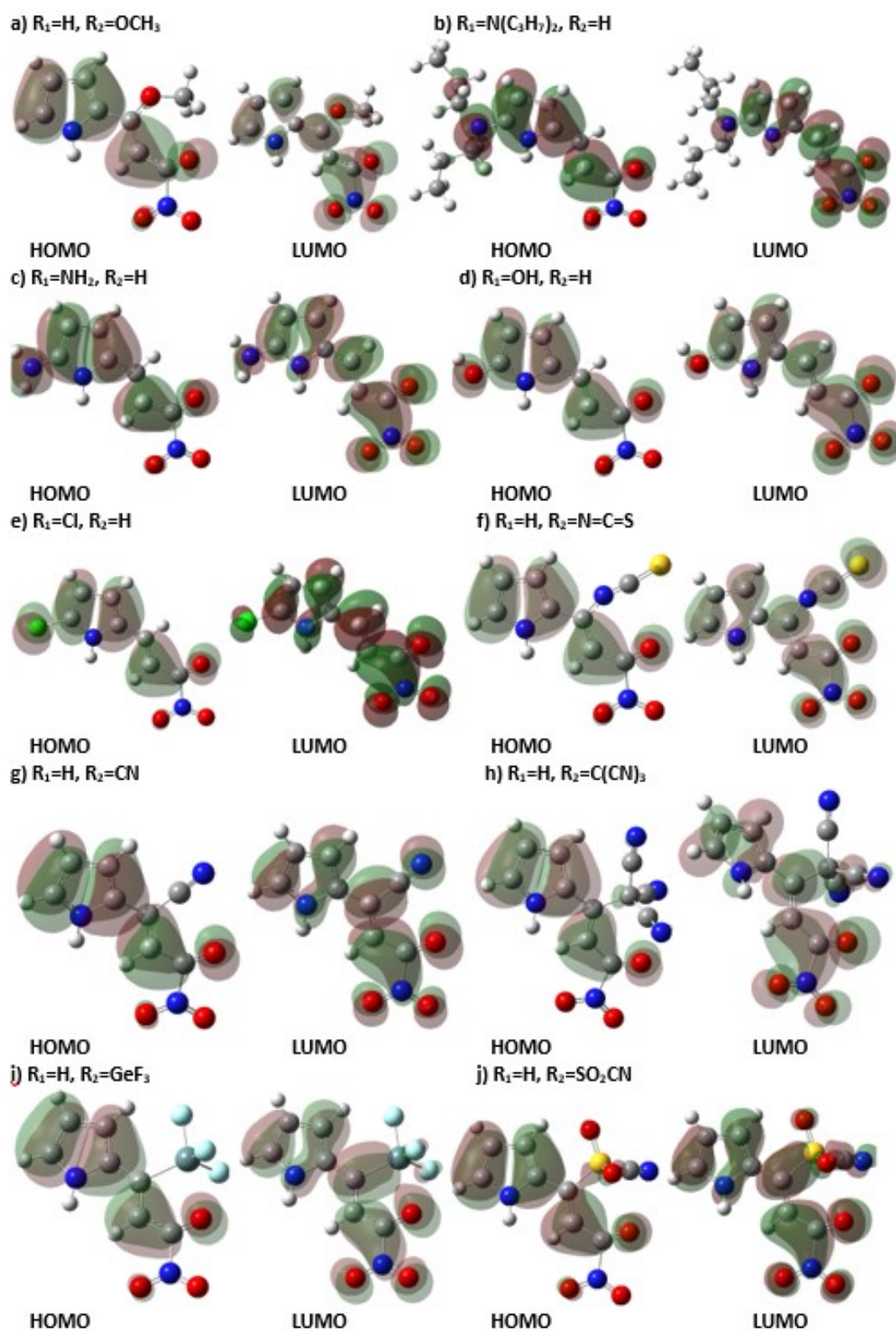
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**Table S1.** The value of Hammett constants<sup>a</sup> for the  $R_1$ ,  $R_2$  and  $R_3$  substituents for studied pyrrolylenones **1–111**

Substituent	Hammett constants, $\sigma_p$
$N(C_3H_7)_2$	-0.93
$N(CH_3)_2$	-0.83
$NHCH_3$	-0.70
$NH_2$	-0.66
$NHNH_2$	-0.55
$OH$	-0.37
$OCH_3$	-0.27
$CH_3$	-0.17
$CH_2C_6H_5$	-0.09
$H$	0.00
$F$	0.06
$SH$	0.15
$Cl$	0.23
$N=C=S$	0.38
$CHO$	0.42
$CCl_3$	0.46
$CF_3$	0.54
$SiCl_3$	0.56
$CN$	0.66
$NO_2$	0.78
$P(O)Cl_2$	0.90
$C(CN)_3$	0.96
$GeF_3$	0.97
$SO_2Cl$	1.11
$SO_2CN$	1.26
$N\equiv N^{\oplus}$	1.91

<sup>a</sup>Taken from ref. C.Hansch, A. Leo and R.W. Taft, *Chem. Rev.*, 1991, **91**, 165–195.



**Fig. S1** Frontier orbitals of pyrrolylenones 13 (a), 17 (b), 19 (c) and 20 (d), 22 (e), 29 (f), 45 (g), 61 (h), 69 (i), 77 (j)

Equations to Figure 3:

Part a)

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied  
HOMO (energy) =  $-0.42 \times \sigma_p - 5.70$ ,  $r=0.946$  (S1)

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied  
HOMO (energy) =  $-0.42 \times \sigma_p - 5.84$ ,  $r=0.943$  (S2)

3.  $R_1=NH_2$ ,  $R_2$  varied  
HOMO (energy) =  $-0.39 \times \sigma_p - 6.16$ ,  $r=0.931$  (S3)

4.  $R_1=OH$ ,  $R_2$  varied  
HOMO (energy) =  $-0.44 \times \sigma_p - 6.48$ ,  $r=0.925$  (S4)

5.  $R_1=H$ ,  $R_2$  varied  
HOMO (energy) =  $-0.45 \times \sigma_p - 6.87$ ,  $r=0.923$  (S5)

6.  $R_1=Cl$ ,  $R_2$  varied  
HOMO (energy) =  $-0.42 \times \sigma_p - 6.89$ ,  $r=0.925$  (S6)

7.  $R_1=CHO$ ,  $R_2$  varied  
HOMO (energy) =  $-0.40 \times \sigma_p - 7.30$ ,  $r=0.895$  (S7)

8.  $R_1=NO_2$ ,  $R_2$  varied  
HOMO (energy) =  $-0.44 \times \sigma_p - 7.63$ ,  $r=0.907$  (S8)

Part b)

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied  
LUMO (energy) =  $-0.75 \times \sigma_p - 2.71$ ,  $r=0.986$  (S9)

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied  
LUMO (energy) =  $-0.77 \times \sigma_p - 2.81$ ,  $r=0.989$  (S10)

3.  $R_1=NH_2$ ,  $R_2$  varied  
LUMO (energy) =  $-0.81 \times \sigma_p - 2.96$ ,  $r=0.991$  (S11)

4.  $R_1=OH$ ,  $R_2$  varied  
LUMO (energy) =  $-0.83 \times \sigma_p - 3.13$ ,  $r=0.986$  (S12)

5.  $R_1=H$ ,  $R_2$  varied  
LUMO (energy) =  $-0.91 \times \sigma_p - 3.27$ ,  $r=0.986$  (S13)

6.  $R_1=Cl$ ,  $R_2$  varied  
LUMO (energy) =  $-0.88 \times \sigma_p - 3.39$ ,  $r=0.987$  (S14)

7.  $R_1=CHO$ ,  $R_2$  varied  
LUMO (energy) =  $-0.82 \times \sigma_p - 3.79$ ,  $r=0.965$  (S15)

8.  $R_1=NO_2$ ,  $R_2$  varied  
LUMO (energy) =  $-0.77 \times \sigma_p - 4.12$ ,  $r=0.986$  (S16)

Part c)

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied  
 $\Delta(\text{HOMO-LUMO}) = -0.15 \times \sigma_p^2 - 0.31 \times \sigma_p + 3.04$ ,  $r=0.941$  (S17)

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied  
 $\Delta(\text{HOMO-LUMO}) = -0.14 \times \sigma_p^2 - 0.33 \times \sigma_p + 3.09$ ,  $r=0.938$  (S18)

3.  $R_1=NH_2$ ,  $R_2$  varied  
 $\Delta(\text{HOMO-LUMO}) = -0.10 \times \sigma_p^2 - 0.43 \times \sigma_p + 3.25$ ,  $r=0.946$  (S19)

4.  $R_1=OH$ ,  $R_2$  varied  
 $\Delta(\text{HOMO-LUMO}) = -0.14 \times \sigma_p^2 - 0.37 \times \sigma_p + 3.41$ ,  $r=0.949$  (S20)

5.  $R_1=H$ ,  $R_2$  varied  
 $\Delta(\text{HOMO-LUMO}) = -0.07 \times \sigma_p^2 - 0.49 \times \sigma_p + 3.64$ ,  $r=0.930$  (S21)

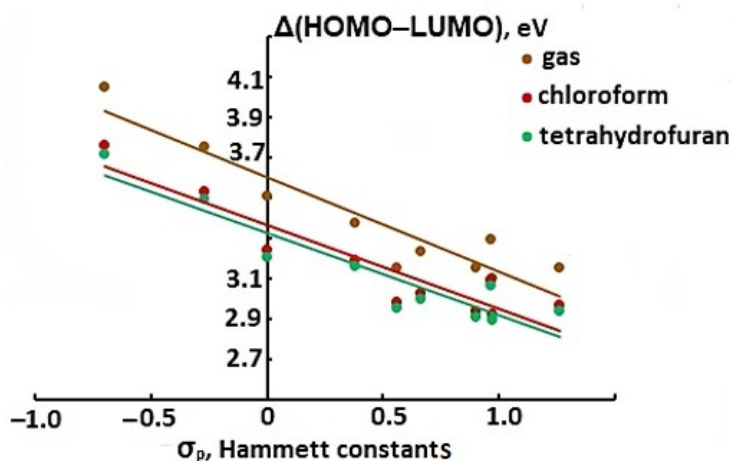
6.  $R_1=Cl$ ,  $R_2$  varied  
 $\Delta(\text{HOMO-LUMO}) = -0.11 \times \sigma_p^2 - 0.47 \times \sigma_p + 3.55$ ,  $r=0.949$  (S22)

7.  $R_1=CHO$ ,  $R_2$  varied  
 $\Delta(\text{HOMO-LUMO}) = -0.10 \times \sigma_p^2 - 0.43 \times \sigma_p + 3.56$ ,  $r=0.940$  (S23)

8.  $R_1=NO_2$ ,  $R_2$  varied  
 $\Delta(\text{HOMO-LUMO}) = -0.16 \times \sigma_p^2 - 0.26 \times \sigma_p + 3.57$ ,  $r=0.935$  (S24)

**Table S2.** The calculated HOMO and LUMO energy (in eV),  $\Delta(\text{HOMO-LUMO})$  gap (in eV),  $\lambda_{\text{max}}$ , absorption wavelength (in nm),  $f$  oscillator strength, main assignment to transition type (HOMO $\rightarrow$  LUMO, contribution in parentheses, %), for pyrrolylenones **5**, **13**, **21**, **29**, **37**, **45**, **53**, **61**, **69**, **77** in gas phase, chloroform ( $\epsilon=4.8$ ), tetrahydrofuran ( $\epsilon=7.6$ ).

No comp	R <sub>2</sub>	$\sigma_p$	gas						chloroform ( $\epsilon=4.8$ )						tetrahydrofuran ( $\epsilon=7.6$ )					
			HOMO	LUMO	gap	$\lambda_{\text{max}}$	f	%	HOMO	LUMO	gap	$\lambda_{\text{max}}$	f	%	HOMO	LUMO	gap	$\lambda_{\text{max}}$	f	%
<b>5</b>	NHCH <sub>3</sub>	-0.7	-6.667	-2.612	4.055	339.39	0.32	95.5	-6.486	-2.722	3.764	382.05	0.28	96.7	-6.466	-2.750	3.716	387.57	0.26	97.2
<b>13</b>	OCH <sub>3</sub>	-0.27	-6.748	-2.993	3.755	353.63	0.39	94.4	-6.562	-3.032	3.529	396.42	0.38	96.8	-6.541	-3.047	3.493	400.72	0.36	96.9
<b>21</b>	H	0	-6.803	-3.293	3.510	366.51	0.46	94.0	-6.525	-3.282	3.242	417.87	0.46	96.3	-6.496	-3.290	3.205	422.79	0.44	96.1
<b>29</b>	N=C=S	0.38	-6.939	-3.565	3.374	376.06	0.43	97.1	-6.688	-3.493	3.194	418.00	0.50	97.3	-6.657	-3.493	3.164	421.38	0.48	96.8
<b>37</b>	SiCl <sub>3</sub>	0.56	-7.021	-3.864	3.157	406.11	0.35	96.2	-6.677	-3.694	2.982	448.81	0.42	98.2	-6.640	-3.685	2.955	452.02	0.40	97.9
<b>45</b>	CN	0.66	-7.238	-4.000	3.238	383.30	0.49	97.2	-6.877	-3.848	3.030	428.75	0.56	97.8	-6.834	-3.835	2.999	431.75	0.54	97.4
<b>53</b>	P(O)Cl <sub>2</sub>	0.9	-7.102	-3.946	3.157	419.31	0.29	96.6	-6.742	-3.803	2.940	465.20	0.35	98.3	-6.702	-3.795	2.907	469.25	0.35	98.2
<b>61</b>	C(CN) <sub>3</sub>	0.96	-7.510	-4.218	3.293	387.04	0.38	94.9	-7.039	-3.945	3.093	429.71	0.45	97.2	-6.975	-3.914	3.062	433.11	0.43	97.2
<b>69</b>	GeF <sub>3</sub>	0.97	-7.374	-4.272	3.102	405.41	0.41	95.6	-6.948	-4.026	2.922	451.25	0.47	97.1	-6.898	-4.003	2.894	454.56	0.46	96.9
<b>77</b>	SO <sub>2</sub> CN	1.26	-7.456	-4.299	3.157	396.29	0.41	96.8	-7.017	-4.047	2.970	437.74	0.49	97.9	-6.963	-4.021	2.942	440.34	0.48	97.7



**Fig. S2.** Dependence of the  $\Delta(\text{HOMO-LUMO})$  gap on the  $\sigma_p$  Hammett constants for pyrrolylenones **5**, **13**, **21**, **29**, **37**, **45**, **53**, **61**, **69**, **77** in the gas phase, chloroform and tetrahydrofuran.

$$\text{gas: } \Delta(\text{HOMO-LUMO}) = -0.47 \times \sigma_p + 3.60, r=0.936 \quad (\text{S25})$$

$$\text{chloroform: } \Delta(\text{HOMO-LUMO}) = -0.42 \times \sigma_p + 3.36, r=0.932 \quad (\text{S26})$$

$$\text{tetrahydrofuran: } \Delta(\text{HOMO-LUMO}) = -0.41 \times \sigma_p + 3.33, r=0.931 \quad (\text{S27})$$

Equations to Figure 5:

1.  $R_1 = \text{N}(\text{C}_3\text{H}_7)_2$ ,  $R_2$  varied

$$\lambda_{\text{max}} = 67.55 \times \sigma_p^2 - 0.92 \times \sigma_p + 408.72, r=0.920 \quad (\text{S28})$$

2.  $R_1 = \text{N}(\text{CH}_3)_2$ ,  $R_2$  varied

$$\lambda_{\text{max}} = 65.27 \times \sigma_p^2 + 1.45 \times \sigma_p + 402.42, r=0.918 \quad (\text{S29})$$

3.  $R_1 = \text{NH}_2$ ,  $R_2$  varied

$$\lambda_{\text{max}} = 60.53 \times \sigma_p^2 + 7.37 \times \sigma_p + 381.64, r=0.916 \quad (\text{S30})$$

4.  $R_1 = \text{OH}$ ,  $R_2$  varied

$$\lambda_{\text{max}} = 53.51 \times \sigma_p^2 + 12.93 \times \sigma_p + 383.98, r=0.921 \quad (\text{S31})$$

5.  $R_1 = \text{H}$ ,  $R_2$  varied

$$\lambda_{\text{max}} = 42.05 \times \sigma_p^2 + 21.84 \times \sigma_p + 351.53, r=0.926 \quad (\text{S32})$$

6.  $R_1 = \text{Cl}$ ,  $R_2$  varied

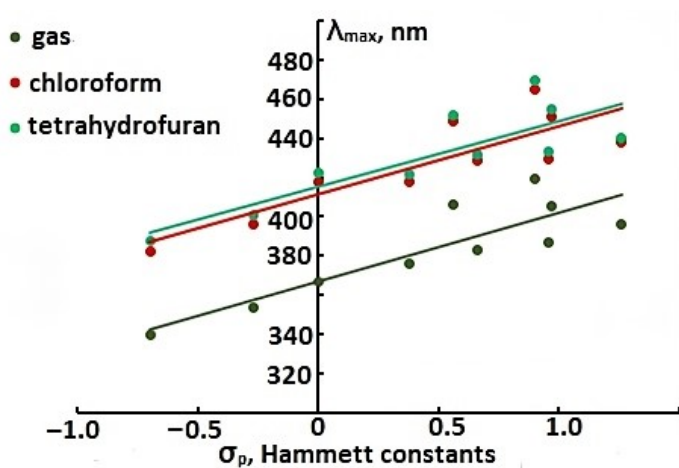
$$\lambda_{\text{max}} = 48.39 \times \sigma_p^2 + 25.58 \times \sigma_p + 354.20, r=0.935 \quad (\text{S33})$$

7.  $R_1 = \text{CHO}$ ,  $R_2$  varied

$$\lambda_{\text{max}} = 32.49 \times \sigma_p^2 + 28.07 \times \sigma_p + 359.05, r=0.930 \quad (\text{S34})$$

8.  $R_1 = \text{NO}_2$ ,  $R_2$  varied

$$\lambda_{\text{max}} = 47.43 \times \sigma_p^2 - 1.45 \times \sigma_p + 358.80, r=0.923 \quad (\text{S35})$$



**Fig. S3.** Dependence of the  $\lambda_{\max}$  wavelength on the  $\sigma_p$  Hammett constants for pyrrolylenones **5, 13, 21, 29, 37, 45, 53, 61, 69, 77** in the gas phase, chloroform and tetrahydrofuran.

$$\text{gas: } \lambda_{\max} = 35.13 \times \sigma_p + 366.72, r=0.874 \quad (\text{S36})$$

$$\text{chloroform: } \lambda_{\max} = 34.67 \times \sigma_p + 411.21, r=0.853 \quad (\text{S37})$$

$$\text{tetrahydrofuran: } \lambda_{\max} = 33.43 \times \sigma_p + 415.57, r=0.841 \quad (\text{S38})$$

Equations to Figure 7:

Part a)

1.  $R_1 = \text{N}(\text{CH}_3)_2$ ,  $R_2$  varied

$$\text{HOMO}(\text{energy}) = -0.03 \times [-E_\pi(\text{PPE})]^2 + 0.49 \times [-E_\pi(\text{PPE})] - 7.88, r=0.979 \quad (\text{S39})$$

2.  $R_1 = \text{NH}_2$ ,  $R_2$  varied

$$\text{HOMO}(\text{energy}) = -0.04 \times [-E_\pi(\text{PPE})]^2 + 0.63 \times [-E_\pi(\text{PPE})] - 8.44, r=0.971 \quad (\text{S40})$$

3.  $R_1 = \text{OH}$ ,  $R_2$  varied

$$\text{HOMO}(\text{energy}) = -0.06 \times [-E_\pi(\text{PPE})]^2 + 0.81 \times [-E_\pi(\text{PPE})] - 8.63, r=0.972 \quad (\text{S41})$$

Part b)

1.  $R_1 = \text{N}(\text{CH}_3)_2$ ,  $R_2$  varied

$$\text{LUMO}(\text{energy}) = -0.03 \times [-E_\pi(\text{PPE})]^2 + 0.49 \times [-E_\pi(\text{PPE})] - 4.45, r=0.978 \quad (\text{S42})$$

2.  $R_1 = \text{NH}_2$ ,  $R_2$  varied

$$\text{LUMO}(\text{energy}) = -0.04 \times [-E_\pi(\text{PPE})]^2 + 0.60 \times [-E_\pi(\text{PPE})] - 4.65, r=0.970 \quad (\text{S43})$$

3.  $R_1 = \text{OH}$ ,  $R_2$  varied

$$\text{LUMO}(\text{energy}) = -0.07 \times [-E_\pi(\text{PPE})]^2 + 0.82 \times [-E_\pi(\text{PPE})] - 4.91, r=0.973 \quad (\text{S44})$$

Part c)

1.  $R_1 = \text{N}(\text{CH}_3)_2$ ,  $R_2$  varied

$$\Delta(\text{HOMO-LUMO}) = -0.09 \times [-E_\pi(\text{PPE})] + 3.98, r=0.941 \quad (\text{S45})$$

2.  $R_1 = \text{NH}_2$ ,  $R_2$  varied

$$\Delta(\text{HOMO-LUMO}) = -0.11 \times [-E_\pi(\text{PPE})] + 4.22, r=0.948 \quad (\text{S46})$$

3.  $R_1 = \text{OH}$ ,  $R_2$  varied

$$\Delta(\text{HOMO-LUMO}) = -0.14 \times [-E_\pi(\text{PPE})] + 4.35, r=0.932 \quad (\text{S47})$$

Equations to Figure 9:

1.  $R_1=N(CH_3)_2$ ,  $R_2$  varied

$$\lambda_{\max} = 1.60 \times [-E_{\pi}(PPE)]^2 - 30.36 \times [-E_{\pi}(PPE)] + 549.75, \quad r=0.961 \quad (S48)$$

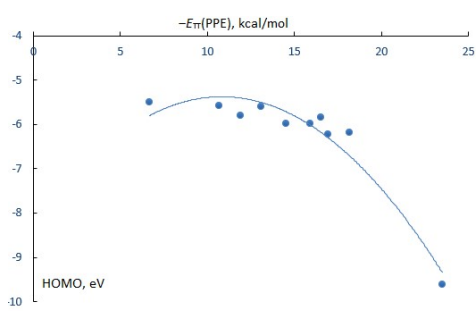
2.  $R_1=NH_2$ ,  $R_2$  varied

$$\lambda_{\max} = 2.07 \times [-E_{\pi}(PPE)]^2 - 32.07 \times [-E_{\pi}(PPE)] + 506.21, \quad r=0.952 \quad (S49)$$

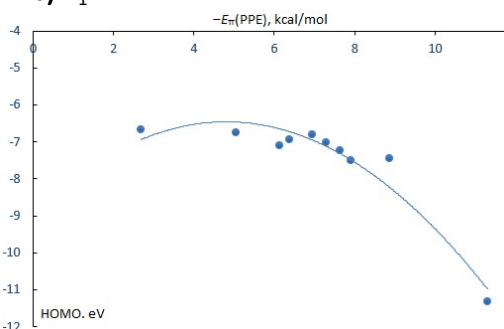
3.  $R_1=OH$ ,  $R_2$  varied

$$\lambda_{\max} = 2.97 \times [-E_{\pi}(PPE)]^2 - 33.87 \times [-E_{\pi}(PPE)] + 456.73, \quad r=0.946 \quad (S50)$$

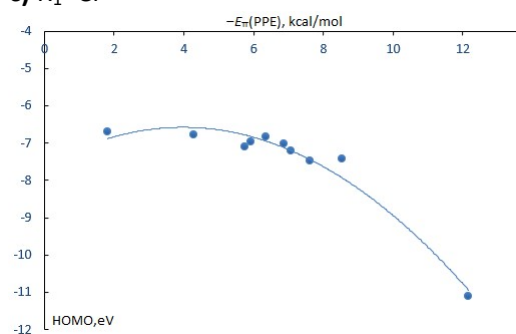
a)  $R_1=N(C_3H_7)_2$



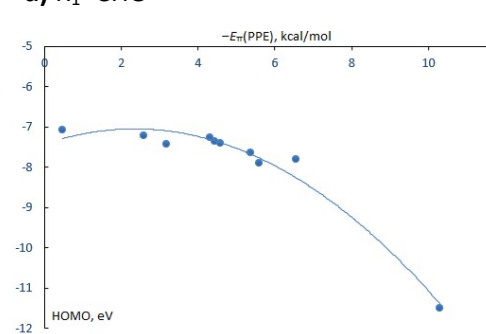
b)  $R_1=H$



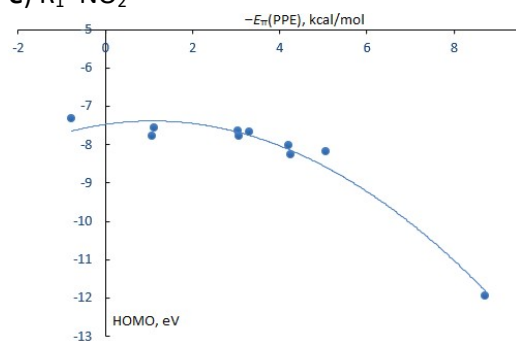
c)  $R_1=Cl$



d)  $R_1=CHO$



e)  $R_1=NO_2$



**Fig. S4** Dependence of the HOMO energy on the  $-E_{\pi}(PPE)$  push-pull effect energy for pyrrolylenones **1, 9, 17, 25, 33, 41, 49, 57, 65, 73, 81**,  $R_1=N(C_3H_7)_2$  (a); **5, 13, 21, 29, 37, 45, 53, 61, 69, 77, 85**,  $R_1=H$  (b); **6, 14, 22, 30, 38, 46, 54, 62, 70, 78, 86**,  $R_1=Cl$  (c); **7, 15, 23, 31, 39, 47, 55, 63, 71, 79, 87**,  $R_1=CHO$  (d); **8, 16, 24, 32, 40, 48, 56, 64, 72, 80, 88**,  $R_1=NO_2$  (e).

Equations to Figure S4:

a)  $R_1=N(C_3H_7)_2$ : HOMO (energy) =  $-0.02 \times [-E_{\pi}(PPE)]^2 + 0.54 \times [-E_{\pi}(PPE)] - 8.26$ ;  $r=0.968$  (S51)

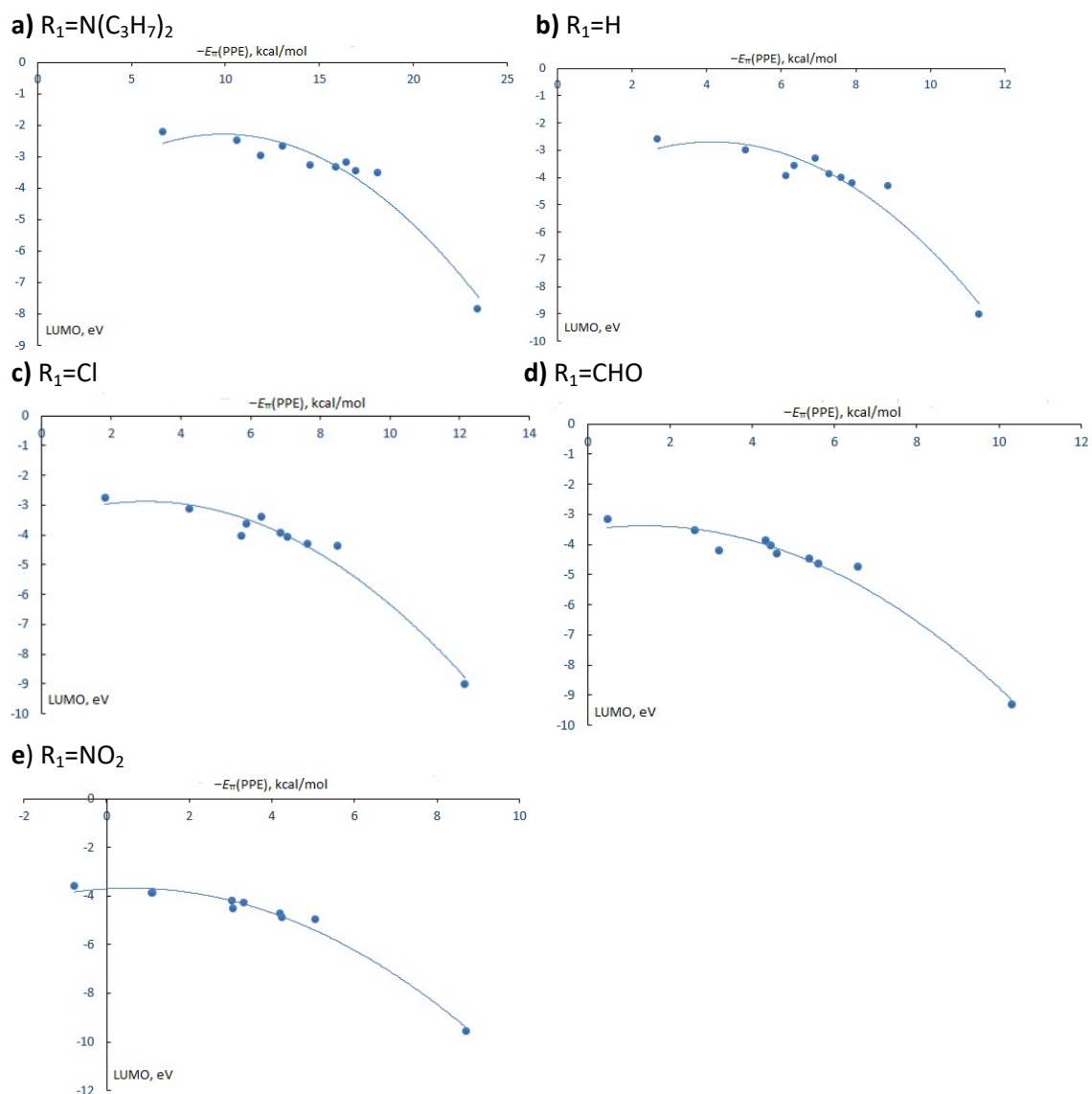
b)  $R_1=H$ : HOMO (energy) =  $-0.11 \times [-E_{\pi}(PPE)]^2 + 1.03 \times [-E_{\pi}(PPE)] - 8.93$ ;  $r=0.965$  (S52)

c)  $R_1=Cl$ : HOMO (energy) =  $-0.07 \times [-E_{\pi}(PPE)]^2 + 0.52 \times [-E_{\pi}(PPE)] - 7.60$ ;  $r=0.984$  (S53)

d)  $R_1=CHO$ : HOMO (energy) =  $-0.07 \times [-E_{\pi}(PPE)]^2 + 0.32 \times [-E_{\pi}(PPE)] - 7.43$ ;  $r=0.986$  (S54)

e)  $R_1=NO_2$ : HOMO (energy) =  $-0.08 \times [-E_{\pi}(PPE)]^2 + 0.16 \times [-E_{\pi}(PPE)] - 7.47$ ;  $r=0.984$  (S55)





**Fig. S5** Dependence of the LUMO energy on the  $-E_{\pi}(\text{PPE})$  push-pull effect energy for pyrrolylenones **1, 9, 17, 25, 33, 41, 49, 57, 65, 73, 81**,  $R_1 = \text{N}(\text{C}_3\text{H}_7)_2$  (a); **5, 13, 21, 29, 37, 45, 53, 61, 69, 77, 85**,  $R_1 = \text{H}$  (b); **6, 14, 22, 30, 38, 46, 54, 62, 70, 78, 86**,  $R_1 = \text{Cl}$  (c); **7, 15, 23, 31, 39, 47, 55, 63, 71, 79, 87**,  $R_1 = \text{CHO}$  (d); **8, 16, 24, 32, 40, 48, 56, 64, 72, 80, 88**,  $R_1 = \text{NO}_2$  (e).

Equations to Figure S5:

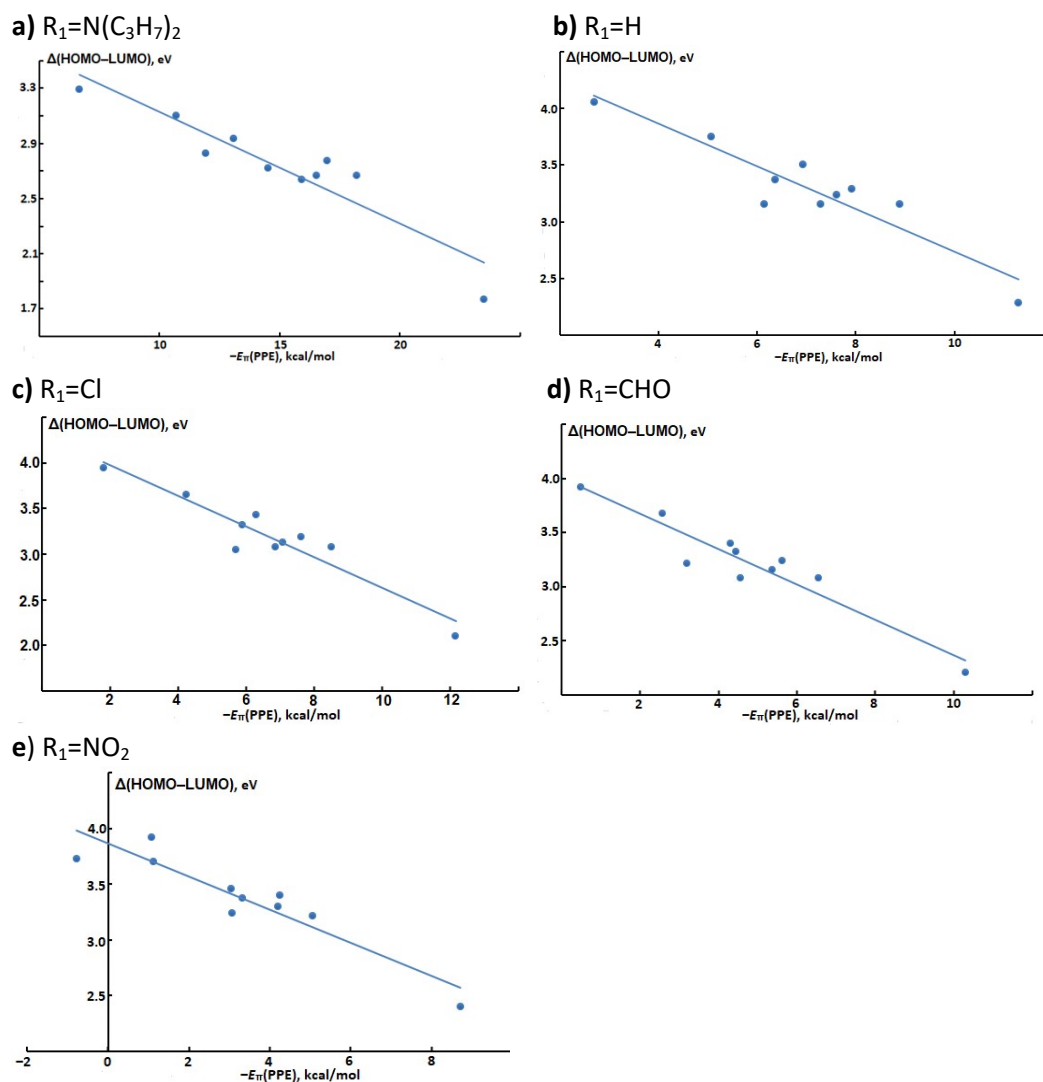
**a)  $R_1 = \text{N}(\text{C}_3\text{H}_7)_2$** :  $\text{LUMO (energy)} = -0.03 \times [-E_{\pi}(\text{PPE})]^2 + 0.56 \times [-E_{\pi}(\text{PPE})] - 5.04$ ;  $r=0.968$  (S56)

**b)  $R_1 = \text{H}$** :  $\text{LUMO (energy)} = -0.12 \times [-E_{\pi}(\text{PPE})]^2 + 0.95 \times [-E_{\pi}(\text{PPE})] - 4.66$ ;  $r=0.962$  (S57)

**c)  $R_1 = \text{Cl}$** :  $\text{LUMO (energy)} = -0.07 \times [-E_{\pi}(\text{PPE})]^2 + 0.42 \times [-E_{\pi}(\text{PPE})] - 3.51$ ;  $r=0.980$  (S58)

**d)  $R_1 = \text{CHO}$** :  $\text{LUMO (energy)} = -0.07 \times [-E_{\pi}(\text{PPE})]^2 + 0.20 \times [-E_{\pi}(\text{PPE})] - 3.52$ ;  $r=0.983$  (S59)

**e)  $R_1 = \text{NO}_2$** :  $\text{LUMO (energy)} = -0.09 \times [-E_{\pi}(\text{PPE})]^2 + 0.10 \times [-E_{\pi}(\text{PPE})] - 3.70$ ;  $r=0.992$  (S60)



**Fig. S6** Dependence of the  $\Delta(\text{HOMO-LUMO})$  gap on the  $-E_{\pi}(\text{PPE})$  push-pull effect energy for pyrrolylenones **1, 9, 17, 25, 33, 41, 49, 57, 65, 73, 81**,  $R_1=\text{N}(\text{C}_3\text{H}_7)_2$  (a); **5, 13, 21, 29, 37, 45, 53, 61, 69, 77, 85**,  $R_1=\text{H}$  (b); **6, 14, 22, 30, 38, 46, 54, 62, 70, 78, 86**,  $R_1=\text{Cl}$  (c); **7, 15, 23, 31, 39, 47, 55, 63, 71, 79, 87**,  $R_1=\text{CHO}$  (d); **8, 16, 24, 32, 40, 48, 56, 64, 72, 80, 88**,  $R_1=\text{NO}_2$  (e).

Equations to Figure S6:

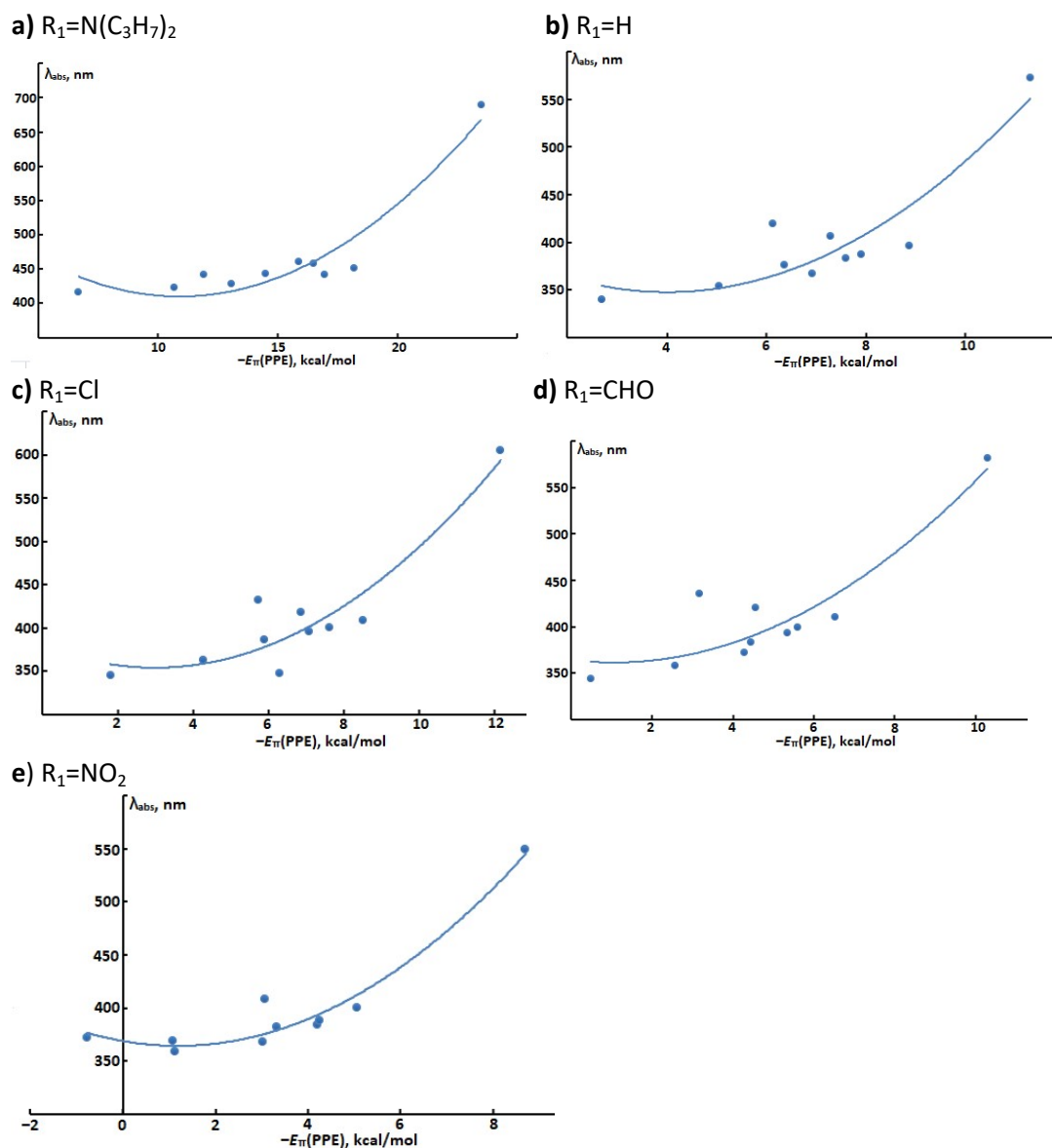
**a)**  $R_1=\text{N}(\text{C}_3\text{H}_7)_2$ :  $\Delta(\text{HOMO-LUMO}) = -0.08 \times [-E_{\pi}(\text{PPE})] + 3.94$ ;  $r=0.929$  (S61)

**b)**  $R_1=\text{H}$ :  $\Delta(\text{HOMO-LUMO}) = -0.19 \times [-E_{\pi}(\text{PPE})] + 4.62$ ;  $r=0.927$  (S62)

**c)**  $R_1=\text{Cl}$ :  $\Delta(\text{HOMO-LUMO}) = -0.17 \times [-E_{\pi}(\text{PPE})] + 4.31$ ;  $r=0.945$  (S63)

**d)**  $R_1=\text{CHO}$ :  $\Delta(\text{HOMO-LUMO}) = -0.16 \times [-E_{\pi}(\text{PPE})] + 4.00$ ;  $r=0.948$  (S64)

**e)**  $R_1=\text{NO}_2$ :  $\Delta(\text{HOMO-LUMO}) = -0.15 \times [-E_{\pi}(\text{PPE})] + 3.86$ ;  $r=0.929$  (S65)



**Fig. S7** Dependence of the  $\lambda_{\max}$  absorption wavelength on the  $-E_{\pi}(\text{PPE})$  push-pull effect energy for pyrrolylenones **1, 9, 17, 25, 33, 41, 49, 57, 65, 73, 81**,  $R_1 = \text{N}(\text{C}_3\text{H}_7)_2$  (a); **5, 13, 21, 29, 37, 45, 53, 61, 69, 77, 85**,  $R_1 = \text{H}$  (b); **6, 14, 22, 30, 38, 46, 54, 62, 70, 78, 86**,  $R_1 = \text{Cl}$  (c); **7, 15, 23, 31, 39, 47, 55, 63, 71, 79, 87**,  $R_1 = \text{CHO}$  (d); **8, 16, 24, 32, 40, 48, 56, 64, 72, 80, 88**,  $R_1 = \text{NO}_2$  (e)..

Equations to Figure S7:

**a)  $R_1 = \text{N}(\text{C}_3\text{H}_7)_2$ :  $\lambda_{\max} = 1.62 \times [-E_{\pi}(\text{PPE})]^2 - 35.34 \times [-E_{\pi}(\text{PPE})] + 602.63$ ;  $r=0.953$  (S66)**

**b)  $R_1 = \text{H}$ :  $\lambda_{\max} = 3.84 \times [-E_{\pi}(\text{PPE})]^2 - 30.76 \times [-E_{\pi}(\text{PPE})] + 409.15$ ;  $r=0.911$  (S67)**

**c)  $R_1 = \text{Cl}$ :  $\lambda_{\max} = 2.85 \times [-E_{\pi}(\text{PPE})]^2 - 17.04 \times [-E_{\pi}(\text{PPE})] + 379.43$ ;  $r=0.929$  (S68)**

**d)  $R_1 = \text{CHO}$ :  $\lambda_{\max} = 2.45 \times [-E_{\pi}(\text{PPE})]^2 - 5.19 \times [-E_{\pi}(\text{PPE})] + 364.10$ ;  $r=0.914$  (S69)**

**e)  $R_1 = \text{NO}_2$ :  $\lambda_{\max} = 3.20 \times [-E_{\pi}(\text{PPE})]^2 - 7.62 \times [-E_{\pi}(\text{PPE})] + 368.75$ ;  $r=0.973$  (S70)**

**The equations used for calculation of photovoltaic performance:**

1) Light-harvesting efficiency (*LHE*):

$$LHE = 1 - 10^{-f} \quad (S71) \quad [24-26, 32]$$

where  $f$  is the oscillator strength

2) Open-circuit voltage ( $V_{OC}$ ):

$$V_{OC} = E_{LUMO} - E_{CB}(TiO_2) \quad (S72) \quad [24-26, 32]$$

where  $E_{CB}(TiO_2)$  – conducting band of  $TiO_2$  (–4.0 eV)

3) Full factor of cell (*FF*):

$$FF = \{(eV_{OC}/K_B T) - \ln[(eV_{OC}/K_B T) + 0.72]\} / [(eV_{OC}/K_B T) + 1] \quad (S73) \quad [30; Ref.S1]$$

where  $e$  is an elementary charge (1),  $K_B$  is Boltzmann constant,  $T$  is temperature at 298K,  $(eV_{OC}/K_B T)$  is the normalized voltage

Ref. S1 L. Zhag, W. Shem, R. He, X. Liu, X. Tang, Y. Yang and M. Li, *Org. Electron.*, 2016, **32**, 134 – 144.

4) The free energy change during the electron-injection process ( $\Delta G_{inject}$ ).

$$\Delta G_{inject} = E^*_{dye} - E_{CB}(TiO_2) \quad (S74) \quad [24 - 26, 31]$$

where  $E^*_{dye}$  is the excited state oxidation potential energy,  $E_{CB}(TiO_2)$  is the reduction potential of the conduction band of the  $TiO_2$  semiconductor;  $E^*_{dye} = E_{dye} - E_{00}$ , where  $E_{dye}$  is oxidation potential energy of the dye in the ground state and  $E_{00}$  is the vertical excitation energy corresponding with  $\lambda_{max}$ .

Driving force of regeneration ( $\Delta G_{regen}$ ) between the oxidized dye and electrolyte.

$$\Delta G_{regen} = E_{redox} - E_{dye} \quad (S75) \quad [24 - 26, 31]$$

where  $E_{redox}$  is the Fermi levels of the iodide/triiodide electrolyte (–4.8 eV),

**Table S3.** The calculated values of light-harvesting efficiency (*LHE*), open-circuit voltage ( $V_{OC}$ , eV), full factor of cell (*FF*), free energy change for the electron-injection process ( $\Delta G_{inject}$ , eV) and driving force of sensitizer regeneration ( $\Delta G_{regen}$ , eV).

No	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	<i>LHE</i>	$V_{OC}$	<i>FF</i>	$\Delta G_{inject}$	$\Delta G_{regen}$
Series ①								
1	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	NHCH <sub>3</sub>	NO <sub>2</sub>	0.532	1.796	0.926	-1.481	0.697
2	N(CH <sub>3</sub> ) <sub>2</sub>			0.521	1.714	0.923	-1.413	0.833
3	NH <sub>2</sub>			0.475	1.605	0.919	-1.250	1.214
4	OH			0.499	1.388	0.909	-1.174	1.486
5	H			0.521	1.388	0.909	-0.987	1.867
6	Cl			0.553	1.252	0.902	-0.898	1.894
7	CHO			0.499	0.843	0.867	-0.533	2.275
8	NO <sub>2</sub>			0.308	0.408	0.775	-0.011	2.52
Series ②								
9	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	OCH <sub>3</sub>	NO <sub>2</sub>	0.628	1.524	0.916	-1.350	0.778
10	N(CH <sub>3</sub> ) <sub>2</sub>			0.611	1.442	0.912	-1.233	0.942
11	NH <sub>2</sub>			0.593	1.306	0.905	-1.111	1.241
12	OH			0.499	1.17	0.896	-0.966	1.568
13	H			0.593	1.007	0.884	-0.758	1.948
14	Cl			0.620	0.871	0.870	-0.647	1.976
15	CHO			0.698	0.462	0.793	-0.260	2.411
16	NO <sub>2</sub>			0.684	0.136	0.557	0.107	2.765
Series ③								
17	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	H	NO <sub>2</sub>	0.718	1.333	0.906	-1.290	0.806
18	N(CH <sub>3</sub> ) <sub>2</sub>			0.698	1.224	0.900	-1.195	0.942
19	NH <sub>2</sub>			0.669	1.088	0.890	-1.043	1.241
20	OH			0.661	0.898	0.873	-0.840	1.595
21	H			0.653	0.707	0.848	-0.580	2.003
22	Cl			0.691	0.599	0.828	-0.735	2.03
23	CHO			0.760	0.136	0.557	-0.071	2.465
24	NO <sub>2</sub>			0.781	-0.191	-	0.276	2.846
Series ④								
25	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	N=C=S	NO <sub>2</sub>	0.771	1.034	0.886	-1.010	0.996
26	N(CH <sub>3</sub> ) <sub>2</sub>			0.743	0.925	0.876	-0.911	1.132
27	NH <sub>2</sub>			0.684	0.707	0.848	-0.681	1.486
28	OH			0.684	0.626	0.834	-0.598	1.758
29	H			0.628	0.435	0.785	-0.358	2.139
30	Cl			0.684	0.354	0.752	-0.243	2.166
31	CHO			0.684	-0.027	-	0.109	2.547
32	NO <sub>2</sub>			0.487	-0.299	-	0.430	2.874
Series ⑤								
33	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	SiCl <sub>3</sub>	NO <sub>2</sub>	0.705	0.816	0.863	-0.855	1.05
34	N(CH <sub>3</sub> ) <sub>2</sub>			0.684	0.707	0.848	-0.757	1.187
35	NH <sub>2</sub>			0.645	0.571	0.822	-0.603	1.459
36	OH			0.611	0.435	0.785	-0.413	1.758
37	H			0.553	0.136	0.557	-0.032	2.221
38	Cl			0.543	0.054	0.344	0.056	2.221
39	CHO			0.553	-0.327	-	0.451	2.602
40	NO <sub>2</sub>			0.583	-0.544	-	0.742	2.983
Series ⑥								
41	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	CN	NO <sub>2</sub>	0.781	0.735	0.852	-0.808	1.187
42	N(CH <sub>3</sub> ) <sub>2</sub>			0.760	0.626	0.834	-0.706	1.323
43	NH <sub>2</sub>			0.725	0.435	0.785	-0.549	1.622
44	OH			0.712	0.245	0.685	-0.307	2.003
45	H			0.676	0	0.329	0.003	2.438
46	Cl			0.712	-0.082	-	0.076	2.411
47	CHO			0.737	-0.49	-	0.493	2.846
48	NO <sub>2</sub>			0.737	-0.735	-	0.796	3.227
Series ⑦								
49	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	P(O)Cl <sub>2</sub>	NO <sub>2</sub>	0.705	0.653	0.839	-0.704	1.187
50	N(CH <sub>3</sub> ) <sub>2</sub>			0.676	0.544	0.816	-0.591	1.323
51	NH <sub>2</sub>			0.628	0.354	0.752	-0.398	1.649
52	OH			0.543	0.218	0.661	-0.150	1.976
53	H			0.487	0.054	0.344	0.145	2.302
54	Cl			0.521	-0.055	-	0.233	2.302
55	CHO			0.397	-0.218	-	0.578	2.629
56	NO <sub>2</sub>			0.149	0.136	0.557	0.423	2.983
Series ⑧								
57	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	C(CN) <sub>3</sub>	NO <sub>2</sub>	0.725	0.544	0.816	-0.576	1.431
58	N(CH <sub>3</sub> ) <sub>2</sub>			0.712	0.435	0.785	-0.456	1.595

59	NH <sub>2</sub>			0.661	0.245	0.685	-0.285	1.894
60	OH			0.628	-0.027	-	-0.005	2.302
61	H			0.583	-0.218	-	0.306	2.71
62	Cl			0.628	-0.299	-	0.383	2.683
63	CHO			0.611	-0.653	-	0.783	3.091
64	NO <sub>2</sub>			0.620	-0.871	-	1.080	3.472
Series ⑨								
65	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	GeF <sub>3</sub>	NO <sub>2</sub>	0.718	0.408	0.775	-0.418	1.431
66	N(CH <sub>3</sub> ) <sub>2</sub>			0.698	0.326	0.738	-0.322	1.568
67	NH <sub>2</sub>			0.661	0.163	0.598	-0.192	1.812
68	OH			0.637	-0.055	-	0.060	2.193
69	H			0.611	-0.272	-	0.315	2.574
70	Cl			0.661	-0.354	-	0.400	2.574
71	CHO			0.698	-0.708	-	0.741	2.955
72	NO <sub>2</sub>			0.705	-0.98	-	1.021	3.309
Series ⑩								
73	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	SO <sub>2</sub> CN	NO <sub>2</sub>	0.755	0.49	0.802	-0.574	1.377
74	N(CH <sub>3</sub> ) <sub>2</sub>			0.737	0.354	0.752	-0.455	1.54
75	NH <sub>2</sub>			0.676	0.163	0.598	-0.283	1.84
76	OH			0.676	-0.055	-	0.004	2.248
77	H			0.611	-0.299	-	0.327	2.656
78	Cl			0.661	-0.354	-	0.397	2.629
79	CHO			0.653	-0.735	-	0.785	3.01
80	NO <sub>2</sub>			0.653	-0.98	-	1.091	3.391
Series ⑪								
81	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	N≡N <sup>⊕</sup>	NO <sub>2</sub>	0.324	-3.837	-	3.806	4.806
82	N(CH <sub>3</sub> ) <sub>2</sub>			0.383	-4.027	-	3.996	5.023
83	NH <sub>2</sub>			0.339	-4.354	-	4.356	5.459
84	OH			0.324	-4.735	-	4.787	6.003
85	H			0.292	-5.034	-	5.154	6.52
86	Cl			0.354	-5.007	-	5.054	6.302
87	CHO			0.354	-5.306	-	5.377	6.711
88	NO <sub>2</sub>			0.354	-5.551	-	5.690	7.146
Series ⑫								
89	H	H	N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	0.842	2.422	0.942	-2.264	0.996
90			N(CH <sub>3</sub> ) <sub>2</sub>	0.766	2.367	0.941	-2.193	1.05
91			NH <sub>2</sub>	0.791	2.286	0.939	-2.184	1.159
92			NHNH <sub>2</sub>	0.822	2.231	0.938	-2.134	1.187
93			OH	0.791	1.986	0.932	-1.927	1.35
94			OCH <sub>3</sub>	0.781	1.932	0.930	-1.851	1.377
95			CH <sub>3</sub>	0.791	1.959	0.931	-1.890	1.241
96			CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	0.791	1.905	0.929	-1.795	1.214
97			H	0.776	1.66	0.921	-1.664	1.377
98			F	0.786	1.551	0.917	-1.546	1.676
99			SH	0.834	1.66	0.921	-1.581	1.486
100			Cl	0.822	1.36	0.908	-1.332	1.731
101			CONH <sub>2</sub>	0.771	1.306	0.905	-1.276	1.431
102			CHO	0.593	0.952	0.879	-0.785	1.568
103			CCl <sub>3</sub>	0.786	1.306	0.905	-1.223	1.622
104			CF <sub>3</sub>	0.796	1.197	0.898	-1.208	1.731
105			SiCl <sub>3</sub>	0.826	0.98	0.881	-0.958	1.758
106			CN	0.796	0.843	0.867	-0.842	1.867
107			P(O)Cl <sub>2</sub>	0.849	0.735	0.852	-0.731	1.976
5 <sup>p</sup>			NO <sub>2</sub>	0.521	1.388	0.909	-0.987	1.867
108			C(CN) <sub>3</sub>	0.838	0.68	0.844	-0.691	2.166
109			GeF <sub>3</sub>	0.830	0.626	0.834	-0.641	2.139
110			SO <sub>2</sub> Cl	0.781	0.462	0.793	-0.450	2.302
111			SO <sub>2</sub> CN	0.852	0.462	0.793	-0.494	2.329

Equations to Figure 13:

**a)**

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied

$$LHE = -0.87 \times [\Delta(\text{HOMO-LUMO})]^2 + 4.87 \times \Delta(\text{HOMO-LUMO}) - 6.04, \quad r=0.942 \quad (\text{S76})$$

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied

$$LHE = -0.81 \times [\Delta(\text{HOMO-LUMO})]^2 + 4.61 \times \Delta(\text{HOMO-LUMO}) - 5.81, \quad r=0.944 \quad (\text{S77})$$

3.  $R_1=NH_2$ ,  $R_2$  varied

$$LHE = -0.49 \times [\Delta(\text{HOMO-LUMO})]^2 + 2.89 \times \Delta(\text{HOMO-LUMO}) - 3.61, \quad r=0.933 \quad (\text{S78})$$

**b)**

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied

$$V_{OC} = 2.02 \times \Delta(\text{HOMO-LUMO}) - 4.79, \quad r=0.945 \quad (\text{S79})$$

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied

$$V_{OC} = 1.94 \times \Delta(\text{HOMO-LUMO}) - 4.74, \quad r=0.935 \quad (\text{S80})$$

3.  $R_1=NH_2$ ,  $R_2$  varied

$$V_{OC} = 1.72 \times \Delta(\text{HOMO-LUMO}) - 4.52, \quad r=0.947 \quad (\text{S81})$$

**c)**

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied

$$FF = -0.30 \times [\Delta(\text{HOMO-LUMO})]^2 + 1.94 \times \Delta(\text{HOMO-LUMO}) - 2.23, \quad r=0.854 \quad (\text{S82})$$

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied

$$FF = -0.30 \times [\Delta(\text{HOMO-LUMO})]^2 + 2.05 \times \Delta(\text{HOMO-LUMO}) - 2.51, \quad r=0.805 \quad (\text{S83})$$

3.  $R_1=NH_2$ ,  $R_2$  varied

$$FF = -0.61 \times [\Delta(\text{HOMO-LUMO})]^2 + 4.21 \times \Delta(\text{HOMO-LUMO}) - 6.28, \quad r=0.810 \quad (\text{S84})$$

**d)**

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied

$$\Delta G_{\text{inject}} = 1.48 \times [\Delta(\text{HOMO-LUMO})]^2 - 10.20 \times \Delta(\text{HOMO-LUMO}) + 16.02, \quad r=0.912 \quad (\text{S85})$$

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied

$$\Delta G_{\text{inject}} = 0.96 \times [\Delta(\text{HOMO-LUMO})]^2 - 7.16 \times \Delta(\text{HOMO-LUMO}) + 11.76, \quad r=0.885 \quad (\text{S86})$$

3.  $R_1=NH_2$ ,  $R_2$  varied

$$\Delta G_{\text{inject}} = 1.19 \times [\Delta(\text{HOMO-LUMO})]^2 - 8.78 \times \Delta(\text{HOMO-LUMO}) + 14.90, \quad r=0.923 \quad (\text{S87})$$

Equations to Figure 14:

**a)**

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied

$$LHE = -2 \cdot 10^{-4} \times \lambda_{\text{max}}^2 + 0.19 \times \lambda_{\text{max}} - 40.84, \quad r=0.927 \quad (\text{S88})$$

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied

$$LHE = -2 \cdot 10^{-4} \times \lambda_{\text{max}}^2 + 0.16 \times \lambda_{\text{max}} - 35.03, \quad r=0.950 \quad (\text{S89})$$

3.  $R_1=NH_2$ ,  $R_2$  varied

$$LHE = -10^{-4} \times \lambda_{\text{max}}^2 + 0.11 \times \lambda_{\text{max}} - 21.78, \quad r=0.934 \quad (\text{S90})$$

**b)**

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied

$$V_{OC} = -2.5 \cdot 10^{-2} \times \lambda_{\text{max}} + 11.97, \quad r=0.886 \quad (\text{S91})$$

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied

$$V_{OC} = -2.4 \cdot 10^{-2} \times \lambda_{\text{max}} + 11.40, \quad r=0.880 \quad (\text{S92})$$

3.  $R_1=NH_2$ ,  $R_2$  varied

$$V_{OC} = -2.3 \cdot 10^{-2} \times \lambda_{\text{max}} + 10.27, \quad r=0.891 \quad (\text{S93})$$

c)

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied

$$FF = -2.5 \cdot 10^{-3} \times \lambda_{\max} + 1.97, \quad r=0.832 \quad (S94)$$

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied

$$FF = -2.9 \cdot 10^{-3} \times \lambda_{\max} + 2.12, \quad r=0.786 \quad (S95)$$

3.  $R_1=NH_2$ ,  $R_2$  varied

$$FF = -4.5 \cdot 10^{-3} \times \lambda_{\max} + 2.63, \quad r=0.726 \quad (S96)$$

d)

1.  $R_1=N(C_3H_7)_2$ ,  $R_2$  varied

$$\Delta G_{\text{inject}} = 1.9 \cdot 10^{-2} \times \lambda_{\max} - 9.34, \quad r=0.880 \quad (S97)$$

2.  $R_1=N(CH_3)_2$ ,  $R_2$  varied

$$\Delta G_{\text{inject}} = 1.8 \cdot 10^{-2} \times \lambda_{\max} - 8.86, \quad r=0.867 \quad (S98)$$

3.  $R_1=NH_2$ ,  $R_2$  varied

$$\Delta G_{\text{inject}} = 1.7 \cdot 10^{-2} \times \lambda_{\max} - 7.70, \quad r=0.880 \quad (S99)$$



## atom coordinates

**1**

7	-2.697500000	0.012760000	-0.530530000
6	-2.484060000	1.453260000	-0.336100000
6	-3.609850000	2.340470000	-0.872430000
6	-3.230650000	3.823230000	-0.799210000
6	-4.029130000	-0.547910000	-0.284460000
6	-4.426920000	-0.653380000	1.195690000
6	-5.807570000	-1.291290000	1.373340000
1	-2.305600000	1.685620000	0.725500000
1	-1.576010000	1.732240000	-0.879420000
1	-3.824110000	2.060600000	-1.909150000
1	-4.528470000	2.178320000	-0.301110000
1	-4.046630000	4.451030000	-1.164120000
1	-3.011270000	4.129070000	0.228000000
1	-2.347330000	4.040340000	-1.406870000
1	-4.757110000	0.061450000	-0.822750000
1	-4.065530000	-1.534090000	-0.753250000
1	-3.671850000	-1.239000000	1.729400000
1	-4.422240000	0.345310000	1.646540000
1	-6.081590000	-1.350920000	2.429310000
1	-6.584120000	-0.713200000	0.862390000
1	-5.830940000	-2.307520000	0.967750000
6	-1.625980000	-0.834510000	-0.367060000
6	-1.585160000	-2.236960000	-0.281950000
6	-0.234470000	-2.614780000	-0.194000000
6	0.550200000	-1.466670000	-0.213010000
7	-0.335030000	-0.390100000	-0.300980000
6	1.972530000	-1.272880000	-0.138510000
6	2.482510000	-0.042460000	0.308530000
6	3.735530000	0.491360000	-0.037980000
7	3.945120000	1.971060000	0.663020000
1	-2.433510000	-2.899490000	-0.267600000
1	0.128860000	-3.623750000	-0.069380000
1	-0.029610000	0.563130000	-0.406910000
1	1.833290000	0.597390000	0.884480000
8	4.648790000	0.151940000	-0.738760000
8	2.992140000	2.504960000	1.221890000
8	5.055660000	2.444930000	0.562900000
7	2.736990000	-2.327680000	-0.506880000
6	4.100750000	-2.604500000	-0.069310000
1	4.249300000	-3.685350000	-0.083040000
1	4.840830000	-2.117410000	-0.704990000
1	4.239800000	-2.242870000	0.951810000
1	2.257760000	-3.065700000	-0.998420000

**2**

6	-2.793840000	0.034550000	-0.111270000
6	-3.000170000	1.398100000	-0.364850000
6	-1.735680000	2.015230000	-0.383200000
6	-0.766910000	1.049480000	-0.134770000
7	-1.448160000	-0.158470000	0.024110000
6	0.667330000	1.127340000	-0.040840000

6	1.437770000	-0.022620000	-0.274040000
6	2.718940000	-0.265060000	0.253140000
7	3.273550000	-1.737300000	-0.235900000
7	-3.698150000	-0.998830000	-0.035740000
1	-3.949260000	1.876010000	-0.538310000
1	-1.545750000	3.054100000	-0.607050000
1	-0.996260000	-1.013930000	0.303820000
7	1.178150000	2.343380000	0.261170000
8	3.465950000	0.317710000	0.989710000
6	-3.270740000	-2.259580000	0.554550000
6	-5.101110000	-0.639670000	0.121720000
1	-4.065410000	-2.994260000	0.427430000
1	-2.390820000	-2.649140000	0.036200000
1	-3.044300000	-2.175820000	1.628170000
1	-5.711930000	-1.530430000	-0.027060000
1	-5.322890000	-0.219660000	1.113460000
1	-5.386920000	0.090010000	-0.637030000
8	2.491930000	-2.518020000	-0.769450000
8	4.444590000	-1.955720000	-0.015190000
1	0.985410000	-0.833790000	-0.821720000
6	2.512730000	2.829720000	-0.071440000
1	0.517190000	3.024200000	0.601200000
1	2.462990000	3.914890000	-0.172110000
1	2.832910000	2.401720000	-1.023990000
1	3.247620000	2.557950000	0.686930000

### 3

6	-3.302040000	-0.882270000	0.117700000
6	-3.790150000	0.360220000	-0.274130000
6	-2.680800000	1.227090000	-0.378830000
6	-1.533820000	0.510370000	-0.060530000
7	-1.948070000	-0.787640000	0.234040000
6	-0.140770000	0.889940000	-0.037260000
6	0.842550000	-0.089990000	-0.225540000
6	2.168130000	-0.016190000	0.244220000
7	3.007460000	-1.369550000	-0.177020000
1	-4.821510000	0.593670000	-0.486710000
1	-2.707470000	2.249200000	-0.724910000
1	-1.350160000	-1.488120000	0.646030000
1	0.548660000	-1.020860000	-0.683410000
8	2.798410000	0.764820000	0.900650000
8	2.400180000	-2.311640000	-0.674600000
8	4.196870000	-1.338530000	0.049500000
7	0.104930000	2.205380000	0.153320000
6	1.298710000	2.935740000	-0.258850000
1	1.016590000	3.975190000	-0.431760000
1	2.089900000	2.882470000	0.489450000
1	1.683010000	2.514630000	-1.190450000
1	-0.677670000	2.754650000	0.473190000
7	-3.965190000	-2.056000000	0.445940000
1	-4.958130000	-2.026810000	0.265310000
1	-3.551720000	-2.905930000	0.084210000

### 4

6	-3.301770000	-0.902880000	0.128300000
6	-3.804760000	0.323640000	-0.276290000
6	-2.690690000	1.187740000	-0.397580000
6	-1.544370000	0.476310000	-0.067870000
7	-1.955070000	-0.816700000	0.244650000
6	-0.150600000	0.866590000	-0.039030000
6	0.840200000	-0.102770000	-0.224310000
6	2.166300000	-0.009400000	0.247130000
7	3.032180000	-1.340400000	-0.179530000
1	-4.838740000	0.556120000	-0.476510000
1	-2.719120000	2.208170000	-0.747730000
1	-1.358070000	-1.553820000	0.589320000
7	0.079010000	2.184650000	0.148770000
8	2.776500000	0.780450000	0.911140000
8	2.450250000	-2.273180000	-0.721100000
8	4.213480000	-1.301680000	0.084630000
1	0.559240000	-1.037670000	-0.682630000
6	1.266140000	2.928690000	-0.257950000
1	-0.709100000	2.724990000	0.470420000
1	0.971710000	3.963660000	-0.436910000
1	1.661440000	2.508360000	-1.185210000
1	2.052950000	2.888240000	0.495760000
8	-3.884820000	-2.086290000	0.412030000
1	-4.839140000	-2.012760000	0.308230000

## 5

6	-3.389980000	-1.649140000	0.322430000
6	-4.083060000	-0.550820000	-0.153270000
6	-3.141080000	0.482140000	-0.358970000
6	-1.887820000	-0.009860000	-0.005560000
7	-2.070540000	-1.315670000	0.401190000
6	-0.573690000	0.613860000	-0.026960000
6	0.559700000	-0.184670000	-0.194360000
6	1.863410000	0.148490000	0.234300000
7	2.928320000	-1.037700000	-0.159890000
1	-5.143600000	-0.507880000	-0.343550000
1	-3.342070000	1.458130000	-0.773540000
1	-1.335490000	-1.902920000	0.764500000
7	-0.572010000	1.956630000	0.097050000
8	2.345220000	1.057530000	0.848520000
8	2.493370000	-2.094120000	-0.603300000
8	4.095340000	-0.775940000	0.029050000
1	0.428280000	-1.175800000	-0.598520000
6	0.471070000	2.873930000	-0.349170000
1	-1.441890000	2.368420000	0.398300000
1	0.004540000	3.836060000	-0.563880000
1	0.927800000	2.489750000	-1.263750000
1	1.256180000	2.996550000	0.397260000
1	-3.736780000	-2.628520000	0.609940000

## 6

6	3.087890000	-0.290070000	0.014270000
6	3.399340000	0.989750000	-0.398230000
6	2.173730000	1.689710000	-0.481930000

6	1.150740000	0.820650000	-0.120670000
7	1.740580000	-0.395860000	0.173670000
6	-0.288940000	1.014790000	-0.041290000
6	-1.136780000	-0.075780000	-0.237590000
6	-2.455910000	-0.183020000	0.258760000
7	-3.143750000	-1.596830000	-0.207560000
17	4.123060000	-1.630560000	0.325840000
1	4.386410000	1.357110000	-0.624570000
1	2.046740000	2.704540000	-0.826250000
1	1.254340000	-1.206830000	0.526690000
1	-0.738970000	-0.948420000	-0.731050000
8	-3.147170000	0.492030000	0.967060000
8	-2.445170000	-2.430010000	-0.772300000
8	-4.319840000	-1.716460000	0.053450000
7	-0.683110000	2.282600000	0.197340000
6	-1.976410000	2.872160000	-0.132640000
1	0.037140000	2.913610000	0.513640000
1	-1.833090000	3.944800000	-0.267380000
1	-2.344970000	2.443850000	-1.067270000
1	-2.720140000	2.687940000	0.642890000

## 7

6	-3.104670000	-0.410100000	0.064640000
6	-3.422630000	0.868870000	-0.386090000
6	-2.222850000	1.588050000	-0.494210000
6	-1.180360000	0.737810000	-0.110640000
7	-1.738840000	-0.466550000	0.217850000
6	0.260790000	0.969450000	-0.038590000
6	1.126970000	-0.105150000	-0.224490000
6	2.456580000	-0.179580000	0.257380000
7	3.167780000	-1.581600000	-0.198280000
1	-4.419510000	1.208420000	-0.617230000
1	-2.108910000	2.596260000	-0.861980000
1	-1.219600000	-1.253150000	0.581470000
7	0.620650000	2.249530000	0.179400000
8	3.136610000	0.519060000	0.952120000
8	2.476160000	-2.438590000	-0.734870000
8	4.350590000	-1.669060000	0.041690000
1	0.741470000	-0.994330000	-0.697950000
6	1.903380000	2.865590000	-0.144820000
1	-0.116500000	2.868590000	0.480480000
1	1.735840000	3.932960000	-0.291280000
1	2.289060000	2.436210000	-1.071980000
1	2.644330000	2.706480000	0.638690000
6	-3.959000000	-1.555230000	0.358130000
8	-5.166120000	-1.551920000	0.248420000
1	-3.420430000	-2.465320000	0.700380000

## 8

6	2.891240000	-0.040760000	0.037240000
6	3.123290000	1.248410000	0.481440000
6	1.861880000	1.868000000	0.543330000
6	0.901710000	0.936480000	0.137250000
7	1.556980000	-0.226230000	-0.164340000

6	-0.553680000	1.059050000	0.023460000
6	-1.341760000	-0.064690000	0.237580000
6	-2.661040000	-0.243620000	-0.254950000
7	-3.303020000	-1.651410000	0.268980000
7	3.810270000	-1.104160000	-0.229600000
1	4.085260000	1.660710000	0.735960000
1	1.659620000	2.867080000	0.896600000
1	1.153640000	-1.077460000	-0.533350000
7	-0.992330000	2.303730000	-0.251390000
8	-3.361130000	0.378180000	-0.999650000
8	3.331200000	-2.161010000	-0.645300000
8	4.999250000	-0.889120000	-0.028930000
8	-2.611660000	-2.377000000	0.971790000
8	-4.439070000	-1.870330000	-0.084950000
1	-0.904500000	-0.906730000	0.751200000
6	-2.320730000	2.844220000	0.019090000
1	-0.294600000	2.956930000	-0.573440000
1	-2.228070000	3.925670000	0.121620000
1	-2.697330000	2.429900000	0.956810000
1	-3.031400000	2.601960000	-0.771220000

**9**

7	-2.707480000	0.044960000	-0.498380000
6	-2.507360000	1.481350000	-0.262640000
6	-3.645950000	2.374610000	-0.760490000
6	-3.280970000	3.857480000	-0.635130000
6	-4.037270000	-0.538730000	-0.293890000
6	-4.441000000	-0.712740000	1.177660000
6	-5.822240000	-1.357880000	1.320810000
1	-2.322430000	1.680750000	0.804280000
1	-1.606390000	1.784020000	-0.805370000
1	-3.862830000	2.131090000	-1.805720000
1	-4.559530000	2.182080000	-0.190640000
1	-4.105000000	4.489300000	-0.973770000
1	-3.060440000	4.128210000	0.401630000
1	-2.402830000	4.105540000	-1.238320000
1	-4.765440000	0.088890000	-0.809950000
1	-4.061680000	-1.502650000	-0.806150000
1	-3.687430000	-1.323320000	1.685220000
1	-4.436840000	0.264110000	1.673870000
1	-6.097790000	-1.468620000	2.372160000
1	-6.597550000	-0.755110000	0.837430000
1	-5.844910000	-2.353140000	0.866400000
6	-1.628230000	-0.792680000	-0.400590000
6	-1.568690000	-2.202590000	-0.451210000
6	-0.222820000	-2.569700000	-0.375450000
6	0.550030000	-1.413530000	-0.261340000
7	-0.348130000	-0.338960000	-0.266090000
6	1.955660000	-1.247300000	-0.151290000
6	2.517110000	-0.026490000	0.228870000
6	3.820920000	0.430080000	-0.045290000
7	4.028160000	1.954230000	0.556420000
1	-2.409090000	-2.869830000	-0.537390000

1	0.174920000	-3.571570000	-0.387480000
1	-0.064930000	0.626240000	-0.268740000
8	2.627450000	-2.368360000	-0.454310000
1	1.866170000	0.696770000	0.694560000
8	4.779420000	0.002560000	-0.622920000
8	3.057960000	2.549500000	1.015140000
8	5.154920000	2.391930000	0.489940000
6	3.893980000	-2.664900000	0.169200000
1	3.969730000	-3.751100000	0.154380000
1	4.709830000	-2.209030000	-0.387040000
1	3.899610000	-2.301170000	1.199000000

## 10

6	-2.800510000	0.051120000	-0.087510000
6	-2.990460000	1.436200000	0.078570000
6	-1.722750000	2.027680000	0.124020000
6	-0.759340000	1.026670000	0.005970000
7	-1.456290000	-0.181980000	-0.107500000
6	0.660930000	1.105320000	0.008550000
6	1.449910000	-0.033480000	0.171150000
6	2.789680000	-0.206730000	-0.232140000
7	3.301150000	-1.733050000	0.130170000
7	-3.722330000	-0.949030000	-0.245420000
1	-3.938840000	1.939280000	0.161200000
1	-1.502660000	3.075190000	0.251520000
1	-1.019280000	-1.064690000	-0.315110000
8	1.099340000	2.360310000	-0.162460000
1	0.967960000	-0.919500000	0.554030000
8	3.612480000	0.461110000	-0.789880000
6	-3.300760000	-2.332820000	-0.070440000
6	-5.114960000	-0.631760000	0.045690000
1	-4.132120000	-2.988140000	-0.327390000
1	-2.479790000	-2.578550000	-0.749580000
1	-2.986600000	-2.553820000	0.959360000
1	-5.746230000	-1.437110000	-0.329930000
1	-5.302890000	-0.506670000	1.121100000
1	-5.403260000	0.285710000	-0.468740000
8	2.482630000	-2.553210000	0.533590000
8	4.480680000	-1.941890000	-0.043600000
6	2.348770000	2.796840000	0.411890000
1	2.235050000	3.870430000	0.553450000
1	2.511570000	2.304930000	1.373230000
1	3.175290000	2.576490000	-0.259470000

## 11

6	3.308780000	-0.890730000	-0.073400000
6	3.787970000	0.408210000	0.113660000
6	2.671220000	1.258100000	0.157150000
6	1.522380000	0.484410000	0.009070000
7	1.950950000	-0.841270000	-0.124450000
6	0.146720000	0.862060000	0.006110000
6	-0.862790000	-0.083960000	0.160700000
6	-2.212390000	0.035710000	-0.236960000

7	-3.039800000	-1.342110000	0.127480000
7	3.993280000	-2.073380000	-0.268200000
1	4.825310000	0.685190000	0.216560000
1	2.674000000	2.325120000	0.309650000
1	1.357440000	-1.603750000	-0.413030000
1	-0.578440000	-1.055290000	0.534000000
8	-2.870520000	0.866340000	-0.792820000
8	-2.415410000	-2.317090000	0.532070000
8	-4.236570000	-1.291230000	-0.044640000
1	3.573620000	-2.907670000	0.118560000
1	4.983700000	-2.022930000	-0.082190000
8	-0.011270000	2.180840000	-0.159440000
6	-1.143140000	2.875820000	0.405360000
1	-1.420110000	2.425010000	1.360620000
1	-1.989560000	2.845510000	-0.276450000
1	-0.799200000	3.897580000	0.557050000

## 12

6	3.312160000	-0.908870000	-0.078160000
6	3.803250000	0.378950000	0.105180000
6	2.679550000	1.226190000	0.159430000
6	1.533520000	0.449330000	0.015690000
7	1.961320000	-0.872240000	-0.125650000
6	0.154840000	0.835920000	0.008040000
6	-0.860500000	-0.099650000	0.154980000
6	-2.212010000	0.042620000	-0.240010000
7	-3.065790000	-1.314010000	0.126750000
1	4.841550000	0.658140000	0.190900000
1	2.681090000	2.294530000	0.300800000
1	1.378230000	-1.670900000	-0.324680000
1	-0.588790000	-1.078540000	0.518340000
8	-2.849750000	0.885890000	-0.798820000
8	-2.463310000	-2.287310000	0.564410000
8	-4.257210000	-1.248320000	-0.073890000
8	0.013070000	2.155880000	-0.150250000
6	-1.112890000	2.865260000	0.409450000
1	-0.751860000	3.878600000	0.576460000
1	-1.951200000	2.857770000	-0.282700000
1	-1.408750000	2.408540000	1.356100000
8	3.916100000	-2.104660000	-0.212790000
1	4.872260000	-1.994630000	-0.179950000

## 13

6	3.404630000	-1.665790000	-0.189970000
6	4.092910000	-0.488040000	0.056980000
6	3.137170000	0.540950000	0.159680000
6	1.877890000	-0.028840000	-0.019620000
7	2.074430000	-1.382790000	-0.230000000
6	0.575440000	0.586590000	0.000460000
6	-0.575700000	-0.172970000	0.135480000
6	-1.893950000	0.196530000	-0.233850000
7	-2.952810000	-1.008010000	0.123330000
1	5.162810000	-0.392890000	0.151700000
1	3.317930000	1.585410000	0.354110000

1	1.347300000	-2.043970000	-0.453610000
1	-0.462890000	-1.193310000	0.467350000
8	-2.389780000	1.142150000	-0.769840000
8	-2.509110000	-2.080050000	0.517250000
8	-4.120650000	-0.738540000	-0.040150000
8	0.658240000	1.912220000	-0.114600000
6	-0.346960000	2.788230000	0.439480000
1	0.177400000	3.718710000	0.649050000
1	-1.152110000	2.944440000	-0.273960000
1	-0.745420000	2.361310000	1.361930000
1	3.765550000	-2.670260000	-0.343090000

#### 14

6	-3.095620000	-0.292850000	0.020370000
6	-3.396970000	1.042810000	-0.179040000
6	-2.165700000	1.726380000	-0.212770000
6	-1.144990000	0.795730000	-0.040150000
7	-1.747870000	-0.446500000	0.098160000
6	0.282510000	0.988650000	-0.006760000
6	1.154730000	-0.076420000	-0.153650000
6	2.514760000	-0.131170000	0.247950000
7	3.176400000	-1.580430000	-0.145350000
17	-4.148950000	-1.644650000	0.172070000
1	-4.386380000	1.454760000	-0.287900000
1	-2.015540000	2.783420000	-0.359300000
1	-1.278320000	-1.312990000	0.312830000
1	0.751160000	-1.003940000	-0.529320000
8	3.253590000	0.605370000	0.829710000
8	2.445270000	-2.452070000	-0.599620000
8	4.365140000	-1.679820000	0.053700000
8	0.594250000	2.273380000	0.167590000
6	1.827800000	2.832100000	-0.335320000
1	1.609920000	3.885190000	-0.502710000
1	2.626600000	2.707910000	0.391340000
1	2.100030000	2.346920000	-1.274620000

#### 15

6	-3.113070000	-0.420760000	0.046150000
6	-3.422860000	0.918070000	-0.195000000
6	-2.217130000	1.627270000	-0.240680000
6	-1.177210000	0.713350000	-0.035180000
7	-1.746430000	-0.522820000	0.135210000
6	0.253530000	0.943730000	-0.001660000
6	1.143990000	-0.102760000	-0.139390000
6	2.513240000	-0.128300000	0.247590000
7	3.200890000	-1.561350000	-0.147050000
1	-4.422140000	1.302610000	-0.321480000
1	-2.081880000	2.682260000	-0.414060000
1	-1.243550000	-1.366540000	0.368130000
1	0.755920000	-1.043340000	-0.498770000
8	3.236870000	0.626490000	0.822380000
8	2.480150000	-2.450410000	-0.583050000
8	4.394100000	-1.631430000	0.032820000
8	0.527340000	2.236080000	0.157390000



6	1.757240000	2.825060000	-0.321450000
1	1.515070000	3.871490000	-0.495300000
1	2.543920000	2.722840000	0.421500000
1	2.059200000	2.344400000	-1.253910000
6	-3.979880000	-1.584700000	0.200960000
8	-5.189240000	-1.546650000	0.135470000
1	-3.448660000	-2.542860000	0.388730000

## 16

6	-2.899710000	-0.035590000	-0.011170000
6	-3.123560000	1.311630000	-0.243100000
6	-1.856120000	1.914660000	-0.262900000
6	-0.899140000	0.917640000	-0.049200000
7	-1.565030000	-0.271900000	0.103780000
6	0.549180000	1.036910000	0.008230000
6	1.356460000	-0.069920000	-0.132510000
6	2.724380000	-0.194910000	0.255470000
7	3.329700000	-1.645120000	-0.187810000
7	-3.828130000	-1.115970000	0.128060000
1	-4.087580000	1.772260000	-0.379670000
1	-1.633820000	2.956430000	-0.424060000
1	-1.180490000	-1.179640000	0.328450000
1	0.902400000	-0.976690000	-0.502520000
8	3.482630000	0.498380000	0.860750000
8	-3.352360000	-2.230110000	0.357090000
8	-5.019370000	-0.858080000	0.011250000
8	2.572320000	-2.448720000	-0.715000000
8	4.503970000	-1.810130000	0.045750000
8	0.909230000	2.305010000	0.185940000
6	2.186800000	2.813090000	-0.260660000
1	2.022790000	3.877130000	-0.417280000
1	2.950350000	2.640570000	0.493230000
1	2.469450000	2.329260000	-1.197550000

## 17

7	-2.477440000	0.081280000	-0.452790000
6	-2.221750000	1.487620000	-0.112410000
6	-3.322550000	2.460770000	-0.541140000
6	-2.898080000	3.913970000	-0.305130000
6	-3.830000000	-0.466340000	-0.300580000
6	-4.238520000	-0.761810000	1.149810000
6	-5.644870000	-1.360910000	1.238310000
1	-2.033420000	1.600860000	0.966690000
1	-1.307610000	1.789840000	-0.632600000
1	-3.546660000	2.305330000	-1.601460000
1	-4.244220000	2.263610000	0.013800000
1	-3.694230000	4.602090000	-0.597300000
1	-2.672580000	4.098060000	0.749480000
1	-2.007900000	4.170360000	-0.886800000
1	-4.532260000	0.235410000	-0.752750000
1	-3.892270000	-1.376110000	-0.900600000
1	-3.509990000	-1.448090000	1.593240000
1	-4.193500000	0.162860000	1.735790000

1	-5.921540000	-1.562640000	2.275660000
1	-6.396030000	-0.682760000	0.821460000
1	-5.709550000	-2.305260000	0.689140000
6	-1.431040000	-0.797440000	-0.451850000
6	-1.425790000	-2.197300000	-0.650750000
6	-0.097600000	-2.619700000	-0.600260000
6	0.726090000	-1.511640000	-0.365480000
7	-0.133930000	-0.408100000	-0.277400000
6	2.120620000	-1.444880000	-0.233140000
6	2.879460000	-0.320280000	-0.015370000
6	4.294370000	-0.433470000	0.102050000
7	4.999380000	1.017440000	0.356040000
1	-2.289780000	-2.816500000	-0.820000000
1	0.259410000	-3.630910000	-0.724570000
1	0.169790000	0.524180000	-0.054930000
1	2.642020000	-2.394640000	-0.312570000
1	2.456610000	0.669530000	0.071610000
8	5.046330000	-1.360570000	0.052480000
8	4.279490000	2.009050000	0.417520000
8	6.204900000	1.010130000	0.467680000

## 18

6	2.677440000	-0.163710000	-0.074320000
6	2.861040000	-1.560860000	-0.025420000
6	1.591420000	-2.142400000	0.002230000
6	0.625030000	-1.129940000	-0.018630000
7	1.334320000	0.077720000	-0.060110000
6	-0.775370000	-1.231110000	0.006430000
6	-1.680750000	-0.199930000	-0.011340000
6	-3.077620000	-0.484740000	0.021780000
7	-3.975620000	0.877800000	-0.005090000
7	3.604620000	0.835840000	-0.155440000
1	3.807450000	-2.073810000	-0.011290000
1	1.369410000	-3.198130000	0.039430000
1	0.904590000	0.987050000	-0.075510000
1	-1.167360000	-2.243570000	0.044230000
1	-1.392260000	0.840000000	-0.050160000
8	-3.700310000	-1.502710000	0.064820000
6	3.192410000	2.212350000	0.083350000
6	4.999790000	0.493580000	0.094590000
1	4.027090000	2.874070000	-0.144330000
1	2.371940000	2.491460000	-0.583450000
1	2.882870000	2.388570000	1.123220000
1	5.629340000	1.322610000	-0.228340000
1	5.198450000	0.289980000	1.155430000
1	5.279150000	-0.384330000	-0.488950000
8	-3.390590000	1.954970000	-0.050600000
8	-5.175870000	0.723630000	0.022300000

## 19

6	-3.344500000	0.534610000	-0.000890000
6	-3.717540000	-0.814180000	0.026660000
6	-2.535100000	-1.565000000	0.018940000
6	-1.444140000	-0.690020000	-0.007710000

7	-1.986940000	0.601840000	-0.015240000
6	-0.067180000	-0.980420000	-0.006680000
6	0.968400000	-0.084040000	-0.001210000
6	2.315180000	-0.561730000	-0.005960000
7	3.394840000	0.659490000	0.006890000
7	-4.127770000	1.663040000	-0.079020000
1	-4.730460000	-1.183200000	0.054890000
1	-2.454820000	-2.641020000	0.046230000
1	-1.451390000	1.448340000	-0.124820000
1	0.826270000	0.986380000	0.010180000
8	2.786150000	-1.657850000	-0.016530000
8	2.964560000	1.807620000	0.016900000
8	4.561220000	0.337200000	0.005760000
1	-3.770060000	2.505980000	0.347350000
1	-5.109610000	1.519470000	0.101950000
1	0.183130000	-2.037630000	-0.012090000

## 20

6	-3.346280000	0.546940000	0.000390000
6	-3.731560000	-0.790760000	0.000250000
6	-2.541710000	-1.539740000	0.000230000
6	-1.455190000	-0.661070000	0.000070000
7	-1.996560000	0.627550000	0.000320000
6	-0.074500000	-0.956640000	-0.000160000
6	0.962670000	-0.068160000	-0.000210000
6	2.309040000	-0.560340000	-0.000430000
8	2.762240000	-1.662640000	-0.000470000
8	-4.047340000	1.693840000	0.000540000
1	-4.744420000	-1.161140000	0.000240000
1	-2.459290000	-2.615820000	0.000190000
1	-1.482280000	1.494760000	0.000370000
1	0.169560000	-2.015420000	-0.000270000
1	0.828700000	1.003440000	-0.000100000
7	3.402450000	0.644210000	-0.000260000
8	4.564110000	0.306340000	-0.000290000
8	2.983920000	1.795830000	-0.000060000
1	-4.991670000	1.503580000	0.000560000

## 21

6	3.649360000	-1.096730000	0.000290000
6	4.158920000	0.193560000	0.000360000
6	3.060330000	1.071310000	0.000260000
6	1.890300000	0.304630000	0.000120000
7	2.290880000	-1.022610000	0.000260000
6	0.540710000	0.746770000	-0.000060000
6	-0.578790000	-0.027880000	-0.000160000
6	-1.872420000	0.600790000	-0.000300000
8	-2.206670000	1.742980000	-0.000300000
1	4.156860000	-2.048330000	0.000330000
1	5.204530000	0.456390000	0.000460000
1	3.088390000	2.150210000	0.000250000
1	1.670550000	-1.816470000	0.000270000
1	0.408120000	1.825120000	-0.000110000
1	-0.557320000	-1.107660000	-0.000100000

7	-3.082530000	-0.484500000	-0.000120000
8	-4.202610000	-0.029250000	-0.000430000
8	-2.780710000	-1.671750000	0.000090000

## 22

6	3.017860000	-0.090500000	-0.000010000
6	3.276500000	1.269950000	0.000070000
6	2.022690000	1.907320000	-0.000010000
6	1.024520000	0.929540000	0.000000000
7	1.675170000	-0.298670000	-0.000010000
6	-0.384590000	1.100290000	0.000000000
6	-1.332480000	0.123780000	0.000010000
6	-2.723370000	0.493250000	-0.000010000
7	-3.703750000	-0.800660000	-0.000020000
17	4.116870000	-1.412250000	-0.000020000
1	4.253330000	1.723850000	0.000140000
1	1.841440000	2.971230000	-0.000010000
1	1.236560000	-1.206550000	-0.000070000
1	-1.103320000	-0.931690000	0.000020000
8	-3.266900000	1.551920000	-0.000030000
8	-3.180520000	-1.908170000	0.000070000
8	-4.890030000	-0.567250000	-0.000010000
1	-0.721890000	2.133100000	-0.000010000

## 23

6	3.042240000	-0.212920000	0.000210000
6	3.304710000	1.158030000	0.000260000
6	2.072170000	1.817190000	0.000140000
6	1.057460000	0.846120000	0.000090000
7	1.679430000	-0.379450000	0.000020000
6	-0.354780000	1.049230000	0.000030000
6	-1.316010000	0.091260000	-0.000080000
6	-2.706350000	0.484870000	-0.000150000
8	-3.224310000	1.554410000	-0.000140000
6	3.955590000	-1.352640000	0.000280000
1	4.291220000	1.592680000	0.000360000
1	1.901720000	2.882960000	0.000140000
1	1.210330000	-1.272830000	-0.000070000
1	-0.672160000	2.088110000	0.000050000
1	-1.106450000	-0.968390000	-0.000120000
7	-3.708310000	-0.787710000	-0.000300000
8	-4.889290000	-0.532640000	-0.000340000
8	-3.201310000	-1.902390000	-0.000290000
8	5.163020000	-1.255690000	0.000360000
1	3.462510000	-2.348740000	0.000160000

## 24

6	2.777010000	0.115770000	-0.000050000
6	2.987280000	1.485510000	-0.000020000
6	1.710990000	2.066010000	0.000460000
6	0.756420000	1.037330000	0.000190000
7	1.444170000	-0.153020000	0.000150000
6	-0.668400000	1.161240000	0.000230000
6	-1.572220000	0.152840000	0.000160000

6	-2.985440000	0.475820000	0.000280000
7	-3.923670000	-0.839330000	-0.000130000
7	3.720550000	-0.961510000	-0.000270000
1	3.948090000	1.972080000	-0.000150000
1	1.480610000	3.120110000	0.000710000
1	1.073560000	-1.093370000	0.000140000
1	-1.041030000	2.181560000	0.000400000
1	-1.305670000	-0.894150000	0.000030000
8	-3.549170000	1.521020000	0.000260000
8	3.255990000	-2.103670000	-0.000260000
8	4.910230000	-0.673220000	-0.000400000
8	-5.115100000	-0.639790000	-0.000150000
8	-3.361560000	-1.926370000	-0.000310000

## 25

7	-3.146410000	-0.123490000	-0.455400000
6	-3.215850000	1.313460000	-0.153110000
6	-4.506220000	2.002060000	-0.603210000
6	-4.418720000	3.519520000	-0.409200000
6	-4.345110000	-0.956910000	-0.307090000
6	-4.700850000	-1.307970000	1.144560000
6	-5.945470000	-2.195650000	1.230360000
1	-3.061900000	1.492440000	0.922430000
1	-2.391090000	1.799750000	-0.683420000
1	-4.687750000	1.771670000	-1.658010000
1	-5.360930000	1.618070000	-0.038930000
1	-5.348970000	4.002570000	-0.715670000
1	-4.240800000	3.779130000	0.638530000
1	-3.608620000	3.952620000	-1.002900000
1	-5.178190000	-0.437940000	-0.782940000
1	-4.192800000	-1.868660000	-0.888060000
1	-3.847560000	-1.812020000	1.609480000
1	-4.865950000	-0.385320000	1.712030000
1	-6.188490000	-2.431730000	2.268840000
1	-6.818490000	-1.704130000	0.789680000
1	-5.796010000	-3.142380000	0.702320000
6	-1.930980000	-0.744080000	-0.419560000
6	-1.603870000	-2.109360000	-0.578960000
6	-0.215930000	-2.220320000	-0.492360000
6	0.324440000	-0.949670000	-0.277040000
7	-0.758330000	-0.065110000	-0.238670000
6	1.676220000	-0.540110000	-0.129540000
6	2.053230000	0.790050000	0.018960000
6	3.381020000	1.239310000	0.197420000
7	3.422940000	2.877610000	0.333430000
1	-2.299620000	-2.913140000	-0.747380000
1	0.364500000	-3.124500000	-0.584800000
1	-0.686380000	0.910730000	-0.008080000
7	2.582100000	-1.566240000	-0.146060000
1	1.298370000	1.559020000	-0.006310000
8	4.447210000	0.704340000	0.269110000
8	2.364080000	3.497220000	0.289280000
8	4.521230000	3.364710000	0.472340000

6	3.666440000	-2.069820000	-0.099990000
16	5.014900000	-2.879930000	-0.059570000

**26**

6	3.141940000	-0.341500000	-0.077750000
6	2.958510000	-1.738670000	-0.061150000
6	1.581800000	-1.976070000	-0.046940000
6	0.914270000	-0.749130000	-0.045630000
7	1.904700000	0.237220000	-0.059110000
6	-0.479040000	-0.463360000	-0.024400000
6	-0.986120000	0.829890000	-0.025840000
6	-2.361430000	1.159410000	0.000150000
7	-2.566780000	2.789080000	-0.008310000
7	4.292610000	0.390150000	-0.134000000
1	3.739530000	-2.479540000	-0.058150000
1	1.094300000	-2.937810000	-0.034000000
1	1.728450000	1.227270000	-0.052540000
7	-1.280770000	-1.571700000	-0.001310000
1	-0.305490000	1.665360000	-0.048330000
8	-3.374490000	0.526850000	0.026430000
6	4.243230000	1.822100000	0.130150000
6	5.554430000	-0.301770000	0.102080000
1	5.221540000	2.252540000	-0.079200000
1	3.528640000	2.314210000	-0.535480000
1	3.978000000	2.051750000	1.171610000
1	6.374400000	0.347130000	-0.204900000
1	5.692880000	-0.572820000	1.157190000
1	5.602270000	-1.208250000	-0.502300000
8	-1.569490000	3.504200000	-0.030010000
8	-3.713140000	3.173300000	0.008400000
6	-2.316350000	-2.171760000	0.019420000
16	-3.584590000	-3.101420000	0.046630000

**27**

7	3.924520000	-2.791850000	-0.128200000
6	3.246140000	-1.600480000	-0.011520000
6	3.731820000	-0.292690000	0.070540000
6	2.619220000	0.561030000	0.076300000
6	1.463000000	-0.215990000	0.005600000
7	1.886340000	-1.548500000	-0.041180000
6	0.086000000	0.164970000	0.009550000
6	-0.958380000	-0.741450000	0.016800000
6	-2.328970000	-0.364330000	-0.004580000
7	-3.294970000	-1.692860000	0.012740000
1	4.771140000	-0.010990000	0.127030000
1	2.642010000	1.636880000	0.147950000
1	1.287550000	-2.339700000	-0.216600000
7	-0.165660000	1.504880000	0.004240000
1	-0.756140000	-1.799180000	0.047990000
8	-2.905160000	0.678060000	-0.032520000
8	-4.484360000	-1.476950000	0.001740000
8	-2.762710000	-2.797960000	0.035090000
6	-0.029270000	2.685810000	-0.006330000
16	0.089400000	4.259720000	-0.021350000

1	4.916620000	-2.740470000	0.046880000
1	3.497180000	-3.610050000	0.282460000

## 28

6	-3.772730000	-0.454550000	-0.000030000
6	-3.864220000	0.933130000	0.000110000
6	-2.542330000	1.414510000	-0.000090000
6	-1.672710000	0.325210000	0.000050000
7	-2.469300000	-0.819610000	-0.000110000
6	-0.240960000	0.299850000	0.000130000
6	0.491130000	-0.873500000	0.000010000
6	1.910140000	-0.937240000	0.000180000
7	2.427890000	-2.489140000	-0.000060000
1	-4.774110000	1.511940000	0.000240000
1	-2.232140000	2.447000000	-0.000120000
1	-2.156090000	-1.777820000	-0.000100000
7	0.335050000	1.538180000	0.000290000
1	-0.022330000	-1.821440000	-0.000210000
8	2.775690000	-0.116070000	0.000370000
8	1.585630000	-3.379850000	-0.000310000
8	3.627000000	-2.641470000	0.000030000
6	1.244290000	2.319290000	0.000090000
16	2.316940000	3.465970000	-0.000240000
8	-4.697780000	-1.429460000	-0.000010000
1	-5.581780000	-1.046730000	-0.000180000

## 29

6	3.790660000	-1.708990000	-0.000100000
6	4.259830000	-0.404960000	0.000080000
6	3.136000000	0.441730000	-0.000030000
6	1.994960000	-0.361360000	-0.000050000
7	2.429390000	-1.674910000	0.000090000
6	0.607080000	0.025330000	-0.000080000
6	-0.425250000	-0.889960000	0.000070000
6	-1.807190000	-0.547120000	-0.000030000
7	-2.745650000	-1.885240000	0.000050000
1	5.296440000	-0.108730000	0.000160000
1	3.130700000	1.519780000	-0.000040000
1	1.837230000	-2.489690000	0.000110000
7	0.407450000	1.373560000	-0.000240000
1	-0.203590000	-1.944870000	0.000260000
8	-2.399320000	0.487340000	-0.000270000
8	-2.190470000	-2.977950000	0.000210000
8	-3.937810000	-1.688810000	-0.000060000
6	-0.231230000	2.388290000	-0.000090000
16	-0.921940000	3.797100000	0.000170000
1	4.323560000	-2.646400000	-0.000150000

## 30

6	-3.465870000	-0.125700000	0.000020000
6	-3.371550000	-1.506050000	-0.000070000
6	-1.997050000	-1.808550000	0.000110000
6	-1.283660000	-0.611300000	0.000010000
7	-2.217340000	0.414110000	0.000020000

6	0.141130000	-0.398050000	-0.000020000
6	0.708720000	0.858860000	-0.000040000
6	2.110950000	1.109250000	-0.000050000
7	2.424620000	2.710950000	-0.000030000
17	-4.859760000	0.878930000	-0.000010000
1	-4.200700000	-2.193610000	-0.000150000
1	-1.552190000	-2.790560000	0.000170000
1	-2.026690000	1.404000000	0.000040000
1	0.075590000	1.731430000	-0.000050000
8	3.071350000	0.403180000	-0.000010000
8	1.472930000	3.483030000	0.000000000
8	3.593760000	3.015470000	0.000060000
7	0.868510000	-1.550750000	0.000020000
6	1.874120000	-2.205800000	0.000000000
16	3.086510000	-3.200160000	-0.000010000

**31**

6	-3.511270000	-0.106420000	-0.000010000
6	-3.462910000	1.287210000	0.000270000
6	-2.114710000	1.659860000	0.000060000
6	-1.345640000	0.488860000	0.000080000
7	-2.217490000	-0.569890000	-0.000080000
6	0.096690000	0.352720000	0.000100000
6	0.724570000	-0.872070000	-0.000040000
6	2.141300000	-1.052500000	0.000000000
7	2.537620000	-2.632460000	-0.000030000
1	-4.327740000	1.930820000	0.000430000
1	-1.711720000	2.659790000	0.000070000
1	-1.962040000	-1.545790000	-0.000120000
7	0.758120000	1.542020000	0.000230000
1	0.137640000	-1.776460000	-0.000170000
8	3.059820000	-0.294340000	0.000180000
8	1.625180000	-3.450160000	-0.000120000
8	3.720440000	-2.875410000	0.000110000
6	1.732180000	2.245730000	0.000060000
16	2.892700000	3.297290000	-0.000220000
6	-4.652180000	-1.017920000	-0.000140000
8	-5.808520000	-0.657270000	-0.000090000
1	-4.390580000	-2.098110000	-0.000400000

**32**

6	-3.230140000	-0.294290000	-0.000020000
6	-3.093360000	-1.671970000	-0.000360000
6	-1.712250000	-1.919970000	-0.000690000
6	-1.048160000	-0.687950000	-0.000490000
7	-2.003830000	0.296210000	-0.000110000
6	0.382330000	-0.430830000	-0.000620000
6	0.900420000	0.841170000	-0.000130000
6	2.301260000	1.138210000	-0.000430000
7	2.573760000	2.738570000	0.000120000
7	-4.408910000	0.518800000	0.000350000
1	-3.902130000	-2.383230000	-0.000370000
1	-1.226590000	-2.882090000	-0.001010000
1	-1.883030000	1.299760000	0.000020000



7	1.134030000	-1.564460000	-0.001220000
1	0.237660000	1.691890000	0.000460000
8	3.272740000	0.449900000	-0.001090000
8	-4.238630000	1.739840000	0.000550000
8	-5.491040000	-0.052810000	0.000410000
8	1.599350000	3.479610000	0.000920000
8	3.734470000	3.071470000	-0.000170000
6	2.169480000	-2.177220000	-0.000080000
16	3.417250000	-3.121070000	0.001180000

**33**

14	2.586310000	-1.359880000	0.179890000
6	-2.462310000	-0.470760000	-0.574150000
6	-2.135740000	-1.835150000	-0.762740000
6	-0.758840000	-1.956470000	-0.627040000
6	-0.197390000	-0.689230000	-0.367040000
7	-1.293940000	0.198750000	-0.364890000
6	1.127590000	-0.204720000	-0.229720000
6	1.344620000	1.167200000	-0.338520000
6	2.576840000	1.841390000	-0.148550000
7	2.413000000	3.448480000	-0.362160000
1	-2.829450000	-2.630960000	-0.973620000
1	-0.203060000	-2.868510000	-0.745840000
1	-1.231770000	1.149390000	-0.042100000
1	0.533450000	1.816610000	-0.630380000
8	3.683760000	1.478380000	0.123560000
8	1.282750000	3.909310000	-0.499550000
8	3.439960000	4.086810000	-0.355470000
17	3.337860000	-0.936540000	2.044550000
17	2.040580000	-3.359790000	0.308840000
17	4.019800000	-1.306160000	-1.287700000
7	-3.669860000	0.142130000	-0.590920000
6	-4.883170000	-0.663710000	-0.764070000
6	-3.778440000	1.593910000	-0.421430000
1	-4.680120000	-1.440410000	-1.507710000
6	-5.423850000	-1.301990000	0.523330000
1	-5.642570000	-0.011040000	-1.202740000
1	-4.698300000	1.908710000	-0.920510000
6	-3.790740000	2.090640000	1.034460000
1	-2.961100000	2.071690000	-0.974430000
6	-6.657800000	-2.167440000	0.254310000
1	-4.634770000	-1.905440000	0.982560000
1	-5.671690000	-0.514310000	1.241530000
6	-3.842870000	3.619080000	1.111490000
1	-4.653190000	1.660050000	1.551800000
1	-2.904950000	1.720320000	1.561680000
1	-7.033610000	-2.610400000	1.179240000
1	-7.470250000	-1.580400000	-0.185220000
1	-6.429150000	-2.985950000	-0.435130000
1	-3.865270000	3.956210000	2.149930000
1	-2.970090000	4.075190000	0.634980000
1	-4.736000000	4.011880000	0.616110000

**34**

14	1.654030000	-1.302190000	0.061170000
6	-3.413470000	-0.261530000	-0.154310000
6	-3.144100000	-1.604460000	-0.497400000
6	-1.762260000	-1.761320000	-0.503420000
6	-1.148900000	-0.534570000	-0.181830000
7	-2.216150000	0.366880000	0.009970000
6	0.197640000	-0.086690000	-0.133300000
6	0.438840000	1.282670000	-0.164290000
6	1.705000000	1.914620000	-0.047860000
7	1.573060000	3.534140000	-0.131260000
1	-3.875200000	-2.364170000	-0.714840000
1	-1.243410000	-2.667660000	-0.757010000
1	-2.101180000	1.283180000	0.410030000
1	-0.378270000	1.967900000	-0.332080000
8	2.819490000	1.503260000	0.087300000
8	0.449750000	4.029370000	-0.117610000
8	2.615410000	4.144180000	-0.187500000
17	2.588000000	-1.021170000	1.868960000
17	1.057010000	-3.289510000	0.115660000
17	2.944170000	-1.186070000	-1.529990000
7	-4.602840000	0.378150000	-0.008150000
6	-5.824320000	-0.416420000	0.060390000
6	-4.634570000	1.738730000	0.512610000
1	-5.818030000	-1.181820000	-0.715760000
1	-6.678870000	0.235320000	-0.120440000
1	-5.639150000	2.140270000	0.387950000
1	-3.954310000	2.381180000	-0.052540000
1	-5.949650000	-0.902670000	1.036080000
1	-4.373210000	1.788970000	1.578650000

### 35

14	0.621770000	-1.541370000	0.035710000
6	-3.772070000	1.179520000	0.027170000
6	-3.992490000	-0.137970000	-0.399910000
6	-2.747580000	-0.763290000	-0.461350000
6	-1.746360000	0.157450000	-0.100700000
7	-2.436440000	1.355390000	0.177270000
6	-0.323900000	0.113320000	-0.092090000
6	0.373140000	1.312490000	-0.106040000
6	1.787060000	1.459770000	-0.035870000
7	2.229690000	3.021260000	-0.079740000
1	-4.952150000	-0.570920000	-0.632910000
1	-2.575190000	-1.775990000	-0.777330000
1	-2.003510000	2.179090000	0.564360000
1	-0.158990000	2.244470000	-0.225630000
8	2.686640000	0.676870000	0.035270000
8	1.354120000	3.874450000	0.026210000
8	3.414280000	3.229290000	-0.200400000
17	1.657710000	-1.636930000	1.806070000
17	-0.639720000	-3.186040000	0.107550000
17	1.810210000	-1.853590000	-1.606170000
7	-4.673680000	2.185010000	0.236710000
1	-5.639430000	1.916960000	0.340250000
1	-4.399040000	2.982660000	0.789180000

**36**

14	0.555950000	-1.557260000	0.042510000
8	-4.512040000	2.348270000	0.348440000
6	-3.722520000	1.310250000	0.034320000
6	-3.993190000	0.035230000	-0.453930000
6	-2.760590000	-0.629960000	-0.522100000
6	-1.743320000	0.239650000	-0.099570000
7	-2.392370000	1.444190000	0.220610000
6	-0.315680000	0.141830000	-0.086560000
6	0.420160000	1.309610000	-0.096510000
6	1.846900000	1.395180000	-0.054790000
7	2.363580000	2.928940000	-0.078720000
1	-4.962200000	-0.354480000	-0.722400000
1	-2.614050000	-1.630150000	-0.887850000
1	-1.970460000	2.241640000	0.672020000
1	-0.078420000	2.262910000	-0.194540000
8	2.703540000	0.565600000	-0.023390000
8	1.529600000	3.816520000	0.058920000
8	3.554390000	3.080790000	-0.218390000
17	1.630780000	-1.679530000	1.786410000
17	-0.790710000	-3.125660000	0.173410000
17	1.682630000	-1.944500000	-1.625660000
1	-5.437120000	2.114470000	0.213940000

**37**

14	-0.649270000	-1.324620000	0.037070000
1	-2.298780000	4.589090000	0.554830000
6	-2.250960000	3.563960000	0.223140000
6	-3.209710000	2.767530000	-0.383560000
6	-2.651840000	1.487640000	-0.537310000
6	-1.339310000	1.516370000	-0.044450000
7	-1.129310000	2.819130000	0.400710000
6	-0.269510000	0.550240000	-0.061770000
6	1.021510000	1.019700000	-0.079350000
6	2.207540000	0.208530000	-0.072010000
7	3.553770000	1.102940000	-0.068760000
1	-4.199470000	3.080600000	-0.674430000
1	-3.129230000	0.641030000	-0.997860000
1	-0.310720000	3.127350000	0.901660000
1	1.208560000	2.081230000	-0.157520000
8	2.371690000	-0.970500000	-0.086020000
8	3.439480000	2.298640000	0.172920000
8	4.582280000	0.508710000	-0.288880000
17	0.165360000	-2.124880000	1.741930000
17	-2.674830000	-1.689880000	0.209020000
17	-0.040270000	-2.291580000	-1.663980000

**38**

14	1.248510000	-1.397960000	0.071050000
17	-5.078900000	0.989170000	0.320560000
6	-3.663030000	0.106980000	-0.087040000
6	-3.538680000	-1.152410000	-0.647500000
6	-2.162300000	-1.428020000	-0.701150000

6	-1.459750000	-0.327250000	-0.193660000
7	-2.429060000	0.612690000	0.162250000
6	-0.056130000	-0.009030000	-0.132430000
6	0.305920000	1.316150000	-0.151500000
6	1.652160000	1.813790000	-0.078740000
7	1.705730000	3.427250000	-0.101530000
1	-4.350110000	-1.782940000	-0.970470000
1	-1.719200000	-2.318020000	-1.111500000
1	-2.257660000	1.469740000	0.665950000
1	-0.445370000	2.081720000	-0.284870000
8	2.705680000	1.261600000	-0.025220000
8	0.652480000	4.030820000	0.063450000
8	2.798380000	3.916390000	-0.262920000
17	2.269630000	-1.160400000	1.833890000
17	0.363120000	-3.258160000	0.231130000
17	2.483500000	-1.497100000	-1.560240000

### 39

14	1.100320000	-1.465800000	0.078010000
6	-3.670330000	0.447590000	-0.012450000
6	-3.632100000	-0.776670000	-0.678920000
6	-2.291500000	-1.158320000	-0.781190000
6	-1.502290000	-0.150520000	-0.199320000
7	-2.375780000	0.819040000	0.246740000
6	-0.065730000	0.040880000	-0.136120000
6	0.399570000	1.326850000	-0.169700000
6	1.789350000	1.716630000	-0.104240000
7	1.972560000	3.315890000	-0.095870000
1	-4.498050000	-1.310560000	-1.035750000
1	-1.917290000	-2.046080000	-1.260810000
1	-2.108810000	1.623150000	0.795870000
1	-0.289790000	2.148450000	-0.307650000
8	2.789840000	1.075760000	-0.074490000
8	0.979270000	3.990430000	0.145680000
8	3.089840000	3.721860000	-0.306870000
17	2.167690000	-1.293200000	1.819660000
17	0.019570000	-3.209250000	0.280260000
17	2.298570000	-1.702210000	-1.564870000
6	-4.804500000	1.267410000	0.406470000
8	-5.962270000	0.981490000	0.194670000
1	-4.535650000	2.201420000	0.945180000

### 40

14	1.457880000	-1.396690000	0.115580000
6	-3.458030000	-0.047090000	-0.167520000
6	-3.285910000	-1.244590000	-0.840100000
6	-1.901070000	-1.456340000	-0.902000000
6	-1.257670000	-0.372950000	-0.283170000
7	-2.247270000	0.483460000	0.149440000
6	0.150610000	-0.021710000	-0.174660000
6	0.471260000	1.303150000	-0.228130000
6	1.818590000	1.833750000	-0.148770000
7	1.849010000	3.437960000	-0.160540000
1	-4.074490000	-1.868870000	-1.225410000

1	-1.410130000	-2.286960000	-1.378810000
1	-2.142630000	1.315330000	0.715040000
1	-0.298830000	2.045000000	-0.393230000
8	2.871280000	1.285930000	-0.098910000
8	0.790080000	4.012830000	0.052610000
8	2.926380000	3.945670000	-0.358200000
17	2.472340000	-1.061310000	1.862980000
17	0.531920000	-3.220300000	0.367840000
17	2.697050000	-1.577090000	-1.502700000
7	-4.657250000	0.621300000	0.238390000
8	-5.724220000	0.114100000	-0.081670000
8	-4.519080000	1.664290000	0.881320000

#### 41

7	-2.658170000	0.101020000	-0.431700000
6	-2.467940000	1.533260000	-0.154290000
6	-3.610610000	2.435630000	-0.625460000
6	-3.254990000	3.914790000	-0.442220000
6	-3.991290000	-0.498500000	-0.289200000
6	-4.417010000	-0.750680000	1.163930000
6	-5.801470000	-1.398810000	1.250510000
1	-2.289630000	1.697160000	0.919230000
1	-1.566470000	1.853600000	-0.685440000
1	-3.819820000	2.230870000	-1.680380000
1	-4.525510000	2.216190000	-0.067850000
1	-4.080660000	4.552910000	-0.763940000
1	-3.045220000	4.148480000	0.605680000
1	-2.374280000	4.190640000	-1.029210000
1	-4.710100000	0.154870000	-0.784920000
1	-4.000830000	-1.433100000	-0.852440000
1	-3.672340000	-1.390440000	1.648350000
1	-4.417720000	0.197980000	1.711910000
1	-6.089860000	-1.569130000	2.290130000
1	-6.569010000	-0.766700000	0.793390000
1	-5.820200000	-2.366190000	0.739420000
6	-1.578170000	-0.725530000	-0.406460000
6	-1.507630000	-2.132080000	-0.559620000
6	-0.166700000	-2.493830000	-0.490250000
6	0.604350000	-1.339160000	-0.289350000
7	-0.299070000	-0.271900000	-0.243260000
6	2.002780000	-1.182890000	-0.150390000
6	2.632590000	0.038610000	0.019440000
6	4.037310000	0.198170000	0.177490000
7	4.423860000	1.783450000	0.357000000
1	-2.341240000	-2.795640000	-0.711400000
1	0.237590000	-3.490120000	-0.580020000
1	-0.043970000	0.678770000	-0.038610000
6	2.745300000	-2.412880000	-0.196290000
1	2.055300000	0.949480000	0.036420000
8	4.959980000	-0.554510000	0.206790000
8	3.516910000	2.610700000	0.340090000
8	5.600080000	2.024240000	0.496900000
7	3.261830000	-3.443950000	-0.246000000

**42**

6	-2.768090000	0.000210000	-0.067950000
6	-2.940620000	1.402100000	-0.044150000
6	-1.671420000	1.975190000	-0.025330000
6	-0.712580000	0.952100000	-0.028920000
7	-1.425540000	-0.251110000	-0.050980000
6	0.701400000	1.022190000	-0.007320000
6	1.531470000	-0.083990000	-0.016100000
6	2.954010000	-0.014880000	0.010700000
7	3.609730000	-1.517530000	-0.006630000
7	-3.697860000	-0.989690000	-0.124280000
1	-3.882530000	1.923230000	-0.039100000
1	-1.439950000	3.028790000	-0.007260000
1	-1.006640000	-1.165510000	-0.042240000
6	1.228770000	2.359020000	0.026520000
1	1.113530000	-1.077900000	-0.044820000
8	3.737730000	0.880820000	0.042300000
6	-3.292850000	-2.374210000	0.083110000
6	-5.098330000	-0.639880000	0.089680000
1	-4.139370000	-3.024550000	-0.131370000
1	-2.491670000	-2.650510000	-0.608160000
1	-2.960320000	-2.565840000	1.112310000
1	-5.722750000	-1.469110000	-0.241520000
1	-5.318100000	-0.429250000	1.144010000
1	-5.360630000	0.234760000	-0.506260000
8	2.851600000	-2.482570000	-0.030770000
8	4.817280000	-1.563400000	0.006740000
7	1.565820000	3.462600000	0.052860000

**43**

6	3.295780000	-0.907020000	-0.003630000
6	3.745740000	0.420400000	0.034570000
6	2.613080000	1.237880000	0.032060000
6	1.473160000	0.424680000	-0.003670000
7	1.935670000	-0.896110000	-0.018860000
6	0.097790000	0.774590000	-0.001610000
6	-0.933270000	-0.142370000	0.005480000
6	-2.316490000	0.211290000	-0.006250000
7	-3.260670000	-1.125590000	0.009510000
7	4.012680000	-2.070270000	-0.085190000
1	4.777740000	0.731270000	0.065420000
1	2.593660000	2.315920000	0.067290000
1	1.355250000	-1.711210000	-0.137280000
6	-0.153380000	2.190160000	-0.006980000
1	-0.722430000	-1.200050000	0.024650000
8	-2.899910000	1.247900000	-0.024750000
8	-2.710310000	-2.222060000	0.025650000
8	-4.452250000	-0.926550000	0.003880000
7	-0.263970000	3.338900000	-0.008750000
1	3.593720000	-2.918300000	0.266940000
1	5.001390000	-1.998190000	0.097940000

**44**

6	-3.296700000	-0.920090000	0.000060000
6	-3.759140000	0.394050000	0.000110000
6	-2.619150000	1.211950000	0.000050000
6	-1.483450000	0.395590000	-0.000020000
7	-1.943600000	-0.921860000	0.000000000
6	-0.103570000	0.752280000	-0.000060000
6	0.928770000	-0.155920000	-0.000060000
6	2.313400000	0.214230000	0.000040000
7	3.275440000	-1.103560000	-0.000010000
1	-4.791380000	0.706050000	0.000160000
1	-2.598870000	2.290480000	0.000050000
1	-1.384020000	-1.760640000	0.000030000
1	0.726810000	-1.215740000	-0.000150000
8	2.875720000	1.261170000	-0.000220000
8	2.738220000	-2.205450000	-0.000680000
8	4.463400000	-0.885630000	0.000820000
6	0.138670000	2.169580000	-0.000060000
7	0.239570000	3.319080000	-0.000080000
8	-3.925460000	-2.103970000	0.000080000
1	-4.880490000	-1.974880000	0.000250000

**45**

6	-3.426980000	-1.646260000	-0.000060000
6	-4.072400000	-0.418390000	0.000060000
6	-3.077960000	0.573470000	0.000000000
6	-1.832970000	-0.065430000	0.000010000
7	-2.084100000	-1.427410000	0.000040000
6	-0.516630000	0.504030000	0.000010000
6	0.638760000	-0.232990000	0.000010000
6	1.955480000	0.346440000	0.000030000
7	3.108480000	-0.804620000	0.000040000
1	-5.139840000	-0.268120000	0.000100000
1	-3.221740000	1.642480000	0.000010000
1	-1.386680000	-2.154280000	0.000070000
1	0.603160000	-1.311330000	0.000020000
8	2.345070000	1.467520000	0.000000000
8	2.744960000	-1.975000000	0.000000000
8	4.247530000	-0.404950000	-0.000170000
6	-0.492740000	1.941160000	0.000020000
7	-0.563750000	3.092920000	0.000020000
1	-3.827210000	-2.647690000	-0.000100000

**46**

6	-3.068330000	-0.323720000	0.000040000
6	-3.347960000	1.033140000	0.000330000
6	-2.107740000	1.692110000	0.000440000
6	-1.095180000	0.728210000	0.000050000
7	-1.721640000	-0.510490000	0.000070000
6	0.327810000	0.901430000	0.000000000
6	1.227780000	-0.131860000	0.000170000
6	2.654570000	0.054820000	0.000040000
7	3.438450000	-1.371460000	0.000050000
17	-4.142500000	-1.661550000	-0.000240000

1	-4.331150000	1.472930000	0.000500000
1	-1.943010000	2.758190000	0.000710000
1	-1.274020000	-1.413860000	-0.000530000
1	0.890540000	-1.156840000	0.000400000
8	3.341090000	1.023040000	-0.000150000
8	2.761150000	-2.392770000	0.000020000
8	4.643830000	-1.306880000	0.000110000
6	0.753110000	2.274150000	-0.000190000
7	1.004230000	3.400390000	-0.000430000

#### 47

6	3.085340000	-0.454150000	-0.000010000
6	3.375180000	0.910480000	0.000020000
6	2.157890000	1.596380000	0.000050000
6	1.126130000	0.643880000	0.000020000
7	1.719810000	-0.594860000	-0.000010000
6	-0.300040000	0.853670000	0.000050000
6	-1.217990000	-0.158770000	0.000170000
6	-2.646130000	0.056740000	0.000170000
7	-3.459370000	-1.348700000	0.000040000
1	4.369450000	1.326920000	0.000040000
1	2.008950000	2.664770000	0.000090000
1	1.238820000	-1.481650000	-0.000140000
1	-0.903390000	-1.191070000	0.000270000
8	-3.305860000	1.041780000	-0.000030000
8	-2.800970000	-2.382050000	-0.000120000
8	-4.662310000	-1.257950000	-0.000040000
6	-0.695750000	2.234290000	-0.000050000
7	-0.927170000	3.364720000	-0.000130000
6	3.976530000	-1.614260000	-0.000060000
8	5.184200000	-1.536250000	-0.000010000
1	3.465800000	-2.600920000	-0.000030000

#### 48

6	2.860220000	-0.061350000	0.000030000
6	3.071520000	1.306870000	0.000400000
6	1.796420000	1.890510000	0.000450000
6	0.844320000	0.860900000	-0.000020000
7	1.527560000	-0.331020000	-0.000090000
6	-0.598120000	0.961670000	-0.000210000
6	-1.432590000	-0.116400000	-0.000380000
6	-2.877560000	-0.002820000	-0.000610000
7	-3.593080000	-1.454770000	0.000080000
7	3.801660000	-1.144450000	-0.000210000
1	4.031530000	1.795020000	0.000630000
1	1.566430000	2.944230000	0.000720000
1	1.163440000	-1.274140000	-0.000420000
6	-1.093280000	2.309480000	-0.000160000
1	-1.041110000	-1.122380000	-0.000340000
8	-3.596600000	0.938940000	-0.000160000
8	3.330680000	-2.283030000	-0.000360000
8	4.990440000	-0.858840000	0.000240000
8	-2.863690000	-2.438070000	0.000230000
8	-4.799250000	-1.444030000	0.000620000



7	-1.398780000	3.422280000	-0.000100000
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**49**

7	-3.451540000	-0.101940000	-0.575320000
6	-4.669730000	-0.916730000	-0.518430000
6	-3.550600000	1.325750000	-0.896960000
6	-2.258210000	-0.667770000	-0.278050000
6	-1.957040000	-1.986550000	0.138620000
6	-0.574430000	-2.093980000	0.221780000
6	0.009290000	-0.855340000	-0.108510000
7	-1.075200000	0.002190000	-0.379310000
1	-4.415920000	-1.931630000	-0.836000000
6	-5.362940000	-0.954230000	0.851210000
1	-5.358630000	-0.523160000	-1.271550000
1	-4.504320000	1.470270000	-1.409210000
6	-3.462180000	2.275470000	0.309080000
1	-2.779630000	1.584270000	-1.634670000
1	-2.671740000	-2.759540000	0.363930000
1	-0.040250000	-2.966030000	0.551700000
1	-0.965880000	0.905520000	-0.811000000
6	1.323790000	-0.324260000	-0.060700000
6	1.503830000	1.046260000	0.053950000
6	2.714040000	1.797530000	0.046780000
7	2.375040000	3.406730000	0.149540000
1	0.628600000	1.653770000	0.226360000
8	3.873590000	1.536180000	0.013850000
8	1.204780000	3.769740000	0.058030000
8	3.330090000	4.131660000	0.297170000
15	2.826020000	-1.361050000	-0.361380000
17	3.824670000	-1.357350000	1.436060000
17	2.267860000	-3.350980000	-0.493300000
8	3.600320000	-0.968460000	-1.548150000
6	-6.593420000	-1.865380000	0.837490000
1	-4.648540000	-1.297040000	1.606330000
1	-5.656370000	0.060500000	1.137960000
6	-3.521770000	3.743970000	-0.120120000
1	-4.281620000	2.050550000	0.998050000
1	-2.536040000	2.087420000	0.860530000
1	-7.080810000	-1.879120000	1.814770000
1	-7.332150000	-1.527920000	0.104020000
1	-6.324070000	-2.896040000	0.587200000
1	-3.467970000	4.404400000	0.747690000
1	-2.688180000	4.002740000	-0.779550000
1	-4.452130000	3.967870000	-0.651230000

**50**

7	-4.373240000	0.520480000	-0.146110000
6	-5.630540000	-0.070950000	0.299030000
6	-4.325710000	1.962410000	-0.362400000
6	-3.220500000	-0.162530000	0.076020000
6	-3.021320000	-1.486910000	0.520840000
6	-1.652540000	-1.737440000	0.482650000
6	-0.981860000	-0.579830000	0.048980000
7	-1.991390000	0.378230000	-0.159540000

1	-5.667430000	-1.123960000	0.018830000
1	-5.768510000	0.012510000	1.384640000
1	-6.455380000	0.436830000	-0.200180000
1	-5.327930000	2.315430000	-0.599000000
1	-3.963590000	2.504370000	0.520690000
1	-3.687390000	2.209190000	-1.215760000
1	-3.787910000	-2.172620000	0.838880000
1	-1.180550000	-2.649420000	0.800730000
1	-1.831400000	1.257540000	-0.623960000
6	0.383870000	-0.191390000	-0.020430000
6	0.720830000	1.148290000	0.053870000
6	2.014710000	1.749810000	-0.006530000
7	1.878600000	3.386220000	0.033400000
1	-0.069480000	1.857170000	0.250100000
8	3.130410000	1.341670000	-0.038980000
8	0.760050000	3.882790000	-0.066630000
8	2.916680000	3.993560000	0.146000000
15	1.736290000	-1.395210000	-0.408320000
17	2.776630000	-1.586310000	1.354420000
17	0.914820000	-3.283940000	-0.600370000
8	2.520480000	-1.056520000	-1.604810000

## 51

7	-3.797650000	3.053820000	0.669530000
6	-3.201060000	1.924020000	0.178890000
6	-3.770420000	0.809790000	-0.451310000
6	-2.752330000	-0.127690000	-0.632590000
6	-1.548080000	0.401710000	-0.138810000
7	-1.873630000	1.687920000	0.334400000
6	-0.183300000	0.000400000	-0.200230000
6	0.806430000	0.963780000	-0.195260000
6	2.224270000	0.787390000	-0.124140000
7	2.983200000	2.238900000	-0.161380000
1	-4.803470000	0.712200000	-0.744720000
1	-2.859580000	-1.072210000	-1.134390000
1	-1.259910000	2.241070000	0.913240000
1	0.503550000	1.996820000	-0.280450000
8	2.945360000	-0.153680000	-0.044940000
8	2.301290000	3.255420000	-0.071460000
8	4.186170000	2.194890000	-0.256440000
15	0.326480000	-1.781580000	-0.310760000
17	1.150860000	-2.157910000	1.536750000
17	-1.367440000	-2.962530000	-0.174970000
8	1.138540000	-2.125920000	-1.486450000
1	-3.248120000	3.899170000	0.720860000
1	-4.755060000	3.207440000	0.393600000

## 52

8	-3.707530000	3.194310000	-0.148510000
6	-3.175980000	1.988640000	0.103370000
6	-3.712000000	0.807580000	0.606280000
6	-2.677420000	-0.140980000	0.576290000
6	-1.518880000	0.465920000	0.076870000
7	-1.869260000	1.798670000	-0.184470000

6	-0.152520000	0.044350000	-0.008810000
6	0.856570000	0.971220000	0.066370000
6	2.278220000	0.742650000	0.046100000
7	3.086700000	2.154490000	-0.042790000
1	-4.723040000	0.659620000	0.950880000
1	-2.748830000	-1.152240000	0.935900000
1	-1.301620000	2.472540000	-0.677050000
1	0.588390000	2.004720000	0.233060000
8	2.954180000	-0.228120000	0.130520000
8	2.440720000	3.168630000	-0.281370000
8	4.281130000	2.086060000	0.120160000
15	0.302270000	-1.713470000	-0.399530000
17	0.893140000	-2.494670000	1.405600000
17	-1.438440000	-2.758970000	-0.764110000
8	1.239250000	-1.859500000	-1.522290000
1	-4.650730000	3.189810000	0.048680000

### 53

1	-2.191580000	4.449000000	-0.144290000
6	-2.147630000	3.393350000	0.071060000
6	-3.102400000	2.539930000	0.598330000
6	-2.550300000	1.245770000	0.604470000
6	-1.250550000	1.327400000	0.098160000
7	-1.031570000	2.665130000	-0.204890000
6	-0.185010000	0.357570000	0.022120000
6	1.114240000	0.750770000	0.143630000
6	2.303290000	-0.078860000	0.205740000
7	3.632590000	0.797090000	-0.107650000
1	-4.085670000	2.823740000	0.937230000
1	-3.023030000	0.353530000	0.979300000
1	-0.221420000	3.018070000	-0.690720000
1	1.316580000	1.803140000	0.293080000
8	2.482940000	-1.209930000	0.501440000
8	3.464650000	1.925220000	-0.555510000
8	4.689010000	0.255890000	0.110300000
15	-0.549740000	-1.420170000	-0.368000000
17	-0.805290000	-2.278340000	1.481170000
17	-2.447290000	-1.472390000	-1.158860000
8	0.419410000	-2.075370000	-1.257150000

### 54

17	-4.672990000	1.700620000	-0.100540000
6	-3.395590000	0.588480000	0.184680000
6	-3.440120000	-0.701020000	0.681950000
6	-2.120180000	-1.187750000	0.646750000
6	-1.289520000	-0.183840000	0.145770000
7	-2.109510000	0.911160000	-0.115040000
6	0.145400000	-0.080840000	0.043270000
6	0.759250000	1.130090000	0.164350000
6	2.181680000	1.416540000	0.203510000
7	2.461270000	2.984070000	-0.099490000
1	-4.321860000	-1.215250000	1.026050000
1	-1.796760000	-2.153800000	0.996260000
1	-1.832240000	1.749750000	-0.603310000

1	0.141300000	2.002250000	0.332960000
8	3.127660000	0.760870000	0.476370000
8	1.520920000	3.645950000	-0.522440000
8	3.586430000	3.371350000	0.100950000
15	1.170260000	-1.568440000	-0.384530000
17	1.646710000	-2.368920000	1.445770000
17	-0.120750000	-2.964660000	-1.168960000
8	2.295890000	-1.309730000	-1.292430000

## 55

6	4.339080000	1.945010000	0.152010000
6	3.343710000	0.918680000	-0.139520000
6	3.490530000	-0.380770000	-0.617950000
6	2.215880000	-0.959540000	-0.672830000
6	1.291080000	-0.000610000	-0.244760000
7	2.000290000	1.135760000	0.063070000
6	-0.161820000	-0.027220000	-0.186700000
6	-0.878790000	1.095840000	-0.419690000
6	-2.335760000	1.269030000	-0.471360000
7	-2.756220000	2.687990000	0.174200000
1	4.430250000	-0.832980000	-0.891370000
1	1.975090000	-1.952370000	-1.016620000
1	1.611580000	1.952960000	0.511820000
1	-0.339350000	2.006620000	-0.656050000
8	-3.192950000	0.625550000	-0.960250000
8	-1.869410000	3.292830000	0.764440000
8	-3.904600000	3.027340000	0.035620000
15	-1.033270000	-1.570300000	0.336000000
17	-0.993060000	-2.746820000	-1.346990000
17	0.272340000	-2.517960000	1.602540000
8	-2.362300000	-1.366700000	0.929650000
8	5.531160000	1.802640000	-0.011200000
1	3.926660000	2.899440000	0.545510000

## 56

7	-4.448080000	-1.012690000	0.129230000
6	-3.322330000	-0.183710000	-0.166860000
6	-3.255970000	1.157450000	-0.492460000
6	-1.889190000	1.455460000	-0.641260000
6	-1.162680000	0.284470000	-0.413340000
7	-2.064890000	-0.709960000	-0.126710000
6	0.267500000	0.001270000	-0.460420000
6	0.762530000	-1.171030000	-0.895110000
6	2.186200000	-1.615550000	-0.956170000
7	2.719350000	-2.216360000	0.424590000
1	-4.098200000	1.818680000	-0.608770000
1	-1.472500000	2.409660000	-0.916920000
1	-1.869500000	-1.649420000	0.192510000
1	0.087970000	-1.904480000	-1.331390000
8	2.855940000	-1.744830000	-1.916520000
8	1.874400000	-2.336640000	1.300650000
8	3.877590000	-2.539540000	0.465200000
15	1.500040000	1.185480000	0.176430000
17	1.349790000	2.861510000	-0.993530000

17	0.788880000	1.803240000	1.984910000
8	2.853130000	0.593370000	0.198140000
8	-4.209470000	-2.188580000	0.417950000
8	-5.559940000	-0.503090000	0.075680000

**57**

6	-1.975540000	-3.072830000	0.386870000
7	-1.664480000	-4.172860000	0.519040000
6	-3.558830000	-1.763490000	-0.777030000
7	-4.324460000	-1.905080000	-1.624320000
6	2.147820000	-0.450030000	-0.558970000
6	1.992420000	-1.848530000	-0.728350000
6	0.648190000	-2.145120000	-0.563540000
6	-0.063240000	-0.953630000	-0.299120000
7	0.907830000	0.069010000	-0.332900000
6	-1.425390000	-0.610100000	-0.154380000
6	-1.837650000	0.704150000	-0.318020000
6	-3.133910000	1.235790000	-0.092840000
7	-3.168080000	2.836670000	-0.380790000
1	2.775790000	-2.552470000	-0.951110000
1	0.222400000	-3.125660000	-0.673670000
1	0.735520000	0.999020000	0.011110000
1	-1.123680000	1.422530000	-0.686810000
8	-4.175230000	0.758800000	0.251830000
8	-4.257090000	3.355760000	-0.324530000
8	-2.107010000	3.407740000	-0.616850000
6	-2.489910000	-1.688600000	0.248320000
6	-3.026230000	-1.356890000	1.593090000
7	-3.349590000	-1.177110000	2.682940000
7	3.265860000	0.306850000	-0.604280000
6	3.195280000	1.764850000	-0.457960000
6	4.571110000	-0.343810000	-0.777410000
1	2.310650000	2.125460000	-0.995400000
6	3.183030000	2.283280000	0.990150000
1	4.055100000	2.182590000	-0.987280000
1	5.238470000	0.394680000	-1.228600000
6	5.194420000	-0.892060000	0.513960000
1	4.462980000	-1.148220000	-1.510960000
6	3.052520000	3.808020000	1.043940000
1	2.361210000	1.818860000	1.546220000
1	4.103130000	1.967640000	1.490670000
6	6.525570000	-1.599180000	0.245310000
1	5.345200000	-0.069920000	1.220260000
1	4.490820000	-1.584200000	0.986810000
1	3.052350000	4.162210000	2.076790000
1	3.883010000	4.296940000	0.525900000
1	2.123010000	4.147830000	0.577670000
1	6.959910000	-1.978450000	1.172750000
1	6.396400000	-2.449450000	-0.431290000
1	7.254730000	-0.921070000	-0.208670000

**58**

6	-0.802680000	-2.985950000	0.139250000
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7	-0.402080000	-4.063330000	0.194300000
6	-2.393210000	-1.697630000	-1.040980000
7	-3.065270000	-1.810370000	-1.968220000
6	3.126820000	0.037690000	-0.148580000
6	3.111150000	-1.332030000	-0.498450000
6	1.787060000	-1.749550000	-0.494060000
6	0.957330000	-0.660000000	-0.154060000
7	1.834050000	0.428380000	0.029920000
6	-0.439690000	-0.442980000	-0.101810000
6	-0.950420000	0.842360000	-0.167450000
6	-2.307350000	1.239820000	-0.020710000
7	-2.464790000	2.851590000	-0.150880000
1	3.968650000	-1.939780000	-0.731170000
1	1.458240000	-2.737800000	-0.759060000
1	1.553650000	1.294950000	0.459260000
1	-0.273710000	1.651670000	-0.389230000
8	-3.324980000	0.641340000	0.166760000
8	-3.598240000	3.267920000	-0.158590000
8	-1.443820000	3.529620000	-0.217310000
6	-1.431380000	-1.643650000	0.086380000
6	-2.113690000	-1.503140000	1.398010000
7	-2.549590000	-1.467890000	2.462630000
7	4.174020000	0.884950000	-0.006380000
6	3.956270000	2.233420000	0.503910000
6	5.527140000	0.337700000	0.031250000
1	3.159120000	2.730080000	-0.055240000
1	4.865300000	2.815270000	0.360330000
1	6.236730000	1.142770000	-0.157090000
1	5.652790000	-0.408570000	-0.753200000
1	3.706480000	2.242290000	1.573360000
1	5.760640000	-0.121580000	0.999420000

## 59

6	-0.812890000	2.715720000	0.112180000
7	-1.587550000	3.564680000	0.169380000
6	1.097480000	2.067280000	-1.125160000
7	1.645390000	2.381600000	-2.086950000
6	-3.362820000	-1.512010000	0.031050000
6	-3.843810000	-0.275900000	-0.424850000
6	-2.758890000	0.596940000	-0.476250000
6	-1.597650000	-0.090300000	-0.073050000
7	-2.021850000	-1.404560000	0.207960000
6	-0.211930000	0.215920000	-0.062290000
6	0.725660000	-0.795880000	-0.106840000
6	2.142360000	-0.663650000	-0.016220000
7	2.876870000	-2.107750000	-0.095010000
1	-4.865440000	-0.056600000	-0.690780000
1	-2.803640000	1.611520000	-0.828790000
1	-1.461360000	-2.076350000	0.710160000
1	0.382460000	-1.805320000	-0.268060000
8	2.870560000	0.276260000	0.092070000
8	4.082660000	-2.079060000	-0.146060000
8	2.173260000	-3.112600000	-0.085040000
6	0.270900000	1.705170000	0.050950000

6	1.009090000	1.877420000	1.327670000
7	1.473070000	2.047410000	2.367040000
7	-4.047250000	-2.648560000	0.349070000
1	-5.014830000	-2.689920000	0.070380000
1	-3.564760000	-3.534090000	0.315730000

**60**

6	-0.868120000	2.678260000	0.148500000
7	-1.663210000	3.505970000	0.230890000
6	1.036790000	2.084320000	-1.129980000
7	1.564190000	2.411740000	-2.098860000
8	-3.932980000	-2.709770000	0.347980000
6	-3.346040000	-1.548000000	0.037110000
6	-3.840140000	-0.344800000	-0.461930000
6	-2.753350000	0.535890000	-0.522760000
6	-1.600020000	-0.131990000	-0.077280000
7	-2.016600000	-1.434410000	0.239850000
6	-0.211800000	0.195970000	-0.058130000
6	0.735960000	-0.797850000	-0.103230000
6	2.157370000	-0.637910000	-0.029060000
7	2.922370000	-2.061580000	-0.093950000
1	-4.859950000	-0.139990000	-0.746060000
1	-2.798310000	1.541020000	-0.901690000
1	-1.463570000	-2.133120000	0.713910000
1	0.408930000	-1.814990000	-0.252920000
8	2.859690000	0.321790000	0.054750000
8	4.126070000	-2.005140000	-0.161510000
8	2.238780000	-3.078010000	-0.058030000
6	0.239860000	1.696440000	0.057830000
6	0.996100000	1.878200000	1.322340000
7	1.476830000	2.052670000	2.353330000
1	-4.884290000	-2.655720000	0.202050000

**61**

6	1.889080000	-1.987270000	0.168100000
7	2.917650000	-2.492350000	0.271890000
6	-0.072870000	-2.052680000	-1.167910000
7	-0.440880000	-2.514200000	-2.155640000
1	3.049820000	3.793430000	0.553910000
6	2.848880000	2.785680000	0.226580000
6	3.676100000	1.854520000	-0.382910000
6	2.936860000	0.671120000	-0.532170000
6	1.647760000	0.896240000	-0.024900000
7	1.631750000	2.216700000	0.415130000
6	0.437090000	0.123580000	-0.035710000
6	-0.776030000	0.753090000	-0.086310000
6	-2.075000000	0.134700000	-0.051710000
7	-3.260470000	1.230500000	-0.079910000
1	4.698940000	2.016280000	-0.682190000
1	3.287550000	-0.231470000	-1.000690000
1	0.874170000	2.640350000	0.928590000
1	-0.793070000	1.825420000	-0.207230000
8	-2.420190000	-1.003670000	-0.022890000
8	-4.375370000	0.791660000	-0.220450000

8	-2.945660000	2.406310000	0.057990000
6	0.514010000	-1.444830000	0.049150000
6	-0.173240000	-1.897760000	1.284130000
7	-0.605710000	-2.243070000	2.293150000

## 62

6	0.087780000	2.906030000	0.211110000
7	-0.494040000	3.892970000	0.317610000
6	1.830040000	1.919410000	-1.063590000
7	2.448660000	2.137590000	-2.008960000
6	-3.352620000	-0.521240000	-0.081530000
6	-3.502480000	0.743940000	-0.625370000
6	-2.221910000	1.315470000	-0.666880000
6	-1.300840000	0.386810000	-0.160200000
7	-2.040480000	-0.748360000	0.173720000
6	0.132760000	0.354000000	-0.091850000
6	0.793650000	-0.842250000	-0.153840000
6	2.213190000	-1.052660000	-0.044600000
7	2.593870000	-2.618900000	-0.118050000
1	-4.429180000	1.187010000	-0.949640000
1	-1.990870000	2.285710000	-1.069870000
1	-1.690520000	-1.548940000	0.678980000
1	0.221820000	-1.737380000	-0.345700000
8	3.127270000	-0.299440000	0.071200000
8	3.771500000	-2.867840000	-0.197750000
8	1.673300000	-3.425640000	-0.071810000
6	0.934050000	1.693880000	0.094740000
6	1.681930000	1.637160000	1.375370000
7	2.171420000	1.643050000	2.416910000
17	-4.542180000	-1.695930000	0.296730000

## 63

6	-0.096730000	2.837060000	0.269760000
7	-0.750040000	3.772740000	0.416310000
6	1.673920000	1.992490000	-1.077120000
7	2.252310000	2.255210000	-2.036540000
6	-3.352000000	-0.722620000	-0.010020000
6	-3.532340000	0.505390000	-0.644800000
6	-2.283060000	1.125760000	-0.727130000
6	-1.331250000	0.261880000	-0.156000000
7	-2.015900000	-0.863210000	0.255070000
6	0.110950000	0.307530000	-0.084280000
6	0.825460000	-0.850420000	-0.157160000
6	2.262460000	-0.990710000	-0.074200000
7	2.716960000	-2.534180000	-0.108870000
1	-4.477410000	0.884440000	-0.998750000
1	-2.080250000	2.077210000	-1.187710000
1	-1.614230000	-1.615520000	0.796240000
1	0.293720000	-1.772330000	-0.339600000
8	3.134200000	-0.186500000	-0.004610000
8	3.898600000	-2.730500000	-0.246150000
8	1.838410000	-3.376740000	0.025280000
6	0.831600000	1.692770000	0.103970000
6	1.623690000	1.665930000	1.358230000



7	2.150880000	1.683370000	2.381020000
6	-4.326910000	-1.745820000	0.374740000
8	-5.512940000	-1.658050000	0.154680000
1	-3.902170000	-2.632410000	0.891530000

#### 64

6	-0.413110000	-2.905530000	0.348200000
7	0.151190000	-3.893310000	0.520330000
6	-2.111670000	-1.932290000	-1.007110000
7	-2.729680000	-2.166350000	-1.949110000
6	3.180260000	0.207250000	-0.152820000
6	3.218890000	-1.023030000	-0.784350000
6	1.893980000	-1.481520000	-0.819390000
6	1.077220000	-0.510540000	-0.218160000
7	1.900690000	0.524610000	0.170520000
6	-0.363210000	-0.387350000	-0.101440000
6	-0.938410000	0.839860000	-0.197850000
6	-2.355350000	1.140710000	-0.101340000
7	-2.646440000	2.717750000	-0.178930000
1	4.100940000	-1.510210000	-1.164740000
1	1.561830000	-2.401120000	-1.269630000
1	1.657700000	1.339490000	0.719030000
1	-0.308490000	1.690880000	-0.413050000
8	-3.301530000	0.431110000	0.000880000
8	-3.805720000	3.031340000	-0.283480000
8	-1.678740000	3.463230000	-0.109630000
6	-1.223880000	-1.679660000	0.151330000
6	-1.988230000	-1.524860000	1.413070000
7	-2.500280000	-1.450720000	2.440970000
7	4.246690000	1.099000000	0.207810000
8	5.380370000	0.781620000	-0.119810000
8	3.927360000	2.118430000	0.820350000

#### 65

7	3.645650000	0.163070000	-0.615140000
6	3.766340000	1.623170000	-0.694030000
6	4.858070000	-0.666770000	-0.667220000
1	2.957650000	2.008740000	-1.326630000
6	3.776250000	2.355400000	0.658080000
1	4.690910000	1.838700000	-1.234360000
1	5.597350000	-0.115960000	-1.254310000
6	5.444530000	-1.034960000	0.702690000
1	4.630710000	-1.573970000	-1.233370000
6	3.848670000	3.874370000	0.478900000
1	2.882580000	2.088730000	1.231800000
1	4.630330000	2.007800000	1.246400000
6	6.674770000	-1.936550000	0.569090000
1	5.710640000	-0.120240000	1.241140000
1	4.675630000	-1.535380000	1.299430000
1	3.859990000	4.379450000	1.446870000
1	4.753940000	4.170150000	-0.059760000
1	2.989210000	4.255070000	-0.081300000
1	7.082870000	-2.186240000	1.550770000

1	6.428850000	-2.875910000	0.064720000
1	7.468510000	-1.448740000	-0.004950000
32	-2.669160000	-1.408360000	0.102640000
6	2.443410000	-0.426430000	-0.454050000
6	2.124080000	-1.812100000	-0.358500000
6	0.755060000	-1.919050000	-0.226240000
6	0.184370000	-0.620020000	-0.227610000
7	1.274960000	0.264780000	-0.371280000
6	-1.126930000	-0.172240000	-0.117750000
6	-1.516600000	1.166670000	-0.142700000
6	-2.890550000	1.401440000	-0.007750000
7	-3.355470000	2.874810000	-0.029550000
1	2.831660000	-2.623180000	-0.383780000
1	0.176360000	-2.823550000	-0.133730000
1	1.191220000	1.266470000	-0.383710000
1	-0.849850000	2.008230000	-0.256470000
8	-3.765560000	0.547740000	0.127800000
8	-2.482570000	3.727480000	-0.154680000
8	-4.544320000	3.075040000	0.079080000
9	-3.709320000	-1.705610000	-1.266690000
9	-1.897510000	-3.013170000	0.094090000
9	-3.388810000	-1.566900000	1.684090000

## 66

7	4.579460000	0.691800000	-0.093660000
6	4.567710000	2.141640000	0.065710000
6	5.843430000	-0.018530000	0.086210000
1	3.884630000	2.603490000	-0.652730000
1	5.564470000	2.527080000	-0.141100000
1	6.652570000	0.600420000	-0.300150000
1	5.834770000	-0.949380000	-0.480010000
32	-1.623150000	-1.388910000	0.010950000
6	3.419750000	-0.001310000	-0.058360000
6	3.206360000	-1.406660000	-0.052010000
6	1.841430000	-1.620730000	-0.041260000
6	1.174820000	-0.370150000	-0.035020000
7	2.200120000	0.599100000	-0.042590000
6	-0.174400000	-0.025730000	-0.021220000
6	-0.661840000	1.278310000	-0.024290000
6	-2.058630000	1.408540000	-0.001410000
7	-2.627460000	2.847780000	-0.004390000
1	3.974760000	-2.160740000	-0.051550000
1	1.329150000	-2.568810000	-0.036670000
1	2.041380000	1.591810000	-0.016950000
1	-0.053260000	2.170020000	-0.044490000
8	-2.874700000	0.492250000	0.020260000
8	-1.811130000	3.762630000	-0.018060000
8	-3.832410000	2.958980000	0.007420000
9	-2.520660000	-1.688030000	-1.453620000
9	-0.730700000	-2.927670000	0.005300000
9	-2.468950000	-1.669200000	1.509340000
1	4.282640000	2.445730000	1.080980000
1	6.041720000	-0.244410000	1.140560000

**67**

7	4.789570000	2.020650000	0.055450000
32	-0.722630000	-1.498420000	0.001650000
6	3.823040000	1.068430000	0.002170000
6	3.964340000	-0.335670000	-0.014630000
6	2.689530000	-0.878220000	-0.014740000
6	1.740980000	0.172570000	0.000070000
7	2.502390000	1.362060000	0.006330000
6	0.345390000	0.180840000	-0.001590000
6	-0.441150000	1.325210000	-0.003980000
6	-1.832580000	1.118230000	0.001500000
7	-2.726330000	2.385630000	-0.003110000
1	4.902690000	-0.867020000	-0.026420000
1	2.424510000	-1.922610000	-0.030880000
1	2.115420000	2.290000000	0.068740000
1	-0.065450000	2.337570000	-0.012830000
8	-2.407450000	0.037880000	0.008960000
8	-2.147150000	3.465700000	-0.009320000
8	-3.922800000	2.208430000	-0.000370000
9	-1.508290000	-1.975930000	-1.478590000
9	0.511400000	-2.774740000	-0.005780000
9	-1.497320000	-1.980930000	1.485770000
1	4.575190000	2.977400000	-0.177250000
1	5.742110000	1.735680000	-0.104410000

**68**

8	-4.659390000	2.147610000	0.000390000
32	0.677870000	-1.522010000	0.000010000
6	-3.794050000	1.129610000	0.000020000
6	-3.975990000	-0.257900000	-0.000420000
6	-2.702200000	-0.823480000	-0.000720000
6	-1.741720000	0.211000000	-0.000050000
7	-2.477320000	1.410500000	0.000160000
6	-0.337520000	0.190360000	0.000060000
6	0.464890000	1.314280000	0.000290000
6	1.862330000	1.092110000	0.001060000
7	2.766470000	2.361060000	-0.000060000
1	-4.923050000	-0.773890000	-0.000660000
1	-2.456770000	-1.872570000	-0.001180000
1	-2.103700000	2.346900000	0.000930000
1	0.103380000	2.331940000	0.000070000
8	2.427140000	0.014290000	0.000650000
8	2.190460000	3.441360000	-0.000640000
8	3.960860000	2.175110000	-0.000580000
9	1.465100000	-1.996490000	1.477320000
9	-0.572460000	-2.774950000	-0.000230000
9	1.465450000	-1.996400000	-1.477150000
1	-5.565820000	1.818780000	0.000410000

**69**

32	0.107780000	-1.482210000	0.000000000
1	3.816260000	3.541740000	-0.000190000
6	3.400640000	2.546060000	-0.000080000
6	4.033430000	1.307440000	0.000150000

6	3.033690000	0.329560000	0.000140000
6	1.782740000	0.978800000	-0.000050000
7	2.061720000	2.346380000	-0.000170000
6	0.457720000	0.476880000	-0.000040000
6	-0.667900000	1.263500000	-0.000030000
6	-1.931090000	0.604920000	-0.000230000
7	-3.189470000	1.538990000	0.000060000
1	5.099120000	1.145310000	0.000300000
1	3.164990000	-0.739400000	0.000270000
1	1.374750000	3.082900000	-0.000430000
1	-0.659720000	2.343600000	0.000070000
8	-2.131800000	-0.586760000	-0.000270000
8	-2.973380000	2.743690000	0.000030000
8	-4.266480000	0.992330000	0.000250000
9	-0.513730000	-2.170530000	-1.468980000
9	1.690220000	-2.256800000	-0.000140000
9	-0.513400000	-2.170220000	1.469280000

## 70

32	1.223940000	-1.476380000	0.000030000
6	-3.653700000	0.318060000	0.000000000
6	-3.583040000	-1.069950000	0.000080000
6	-2.224400000	-1.398340000	-0.000440000
6	-1.471780000	-0.207370000	-0.000130000
7	-2.403950000	0.835860000	-0.000350000
6	-0.076640000	0.031130000	-0.000060000
6	0.495090000	1.280280000	-0.000110000
6	1.917440000	1.345550000	-0.000030000
7	2.540510000	2.779870000	0.000030000
1	-4.425180000	-1.741580000	0.000290000
1	-1.799060000	-2.388210000	-0.000630000
1	-2.198860000	1.822780000	-0.000440000
1	-0.056450000	2.209020000	-0.000230000
8	2.686560000	0.411780000	0.000190000
8	1.751100000	3.715010000	-0.000110000
8	3.746610000	2.843690000	0.000040000
9	2.103720000	-1.764440000	1.469830000
9	0.239650000	-2.939280000	0.000070000
9	2.103790000	-1.764560000	-1.469700000
17	-5.032870000	1.334510000	0.000220000

## 71

32	1.110150000	-1.522220000	0.000020000
6	-3.660750000	0.566880000	-0.000050000
6	-3.651560000	-0.829990000	-0.000420000
6	-2.319720000	-1.240230000	-0.000390000
6	-1.503870000	-0.086780000	-0.000030000
7	-2.364010000	0.997140000	0.000150000
6	-0.085260000	0.067410000	0.000100000
6	0.546430000	1.280430000	0.000320000
6	1.979460000	1.296420000	0.000760000
7	2.643310000	2.719690000	-0.000020000
1	-4.533160000	-1.450280000	-0.000680000
1	-1.949890000	-2.251990000	-0.000620000

1	-2.087210000	1.967010000	0.000480000
1	0.037750000	2.233560000	0.000280000
8	2.716280000	0.345290000	0.000320000
8	1.878050000	3.674490000	-0.000300000
8	3.849830000	2.748990000	-0.000560000
9	1.991880000	-1.823450000	1.463240000
9	0.065220000	-2.933940000	-0.000140000
9	1.992010000	-1.823260000	-1.463170000
6	-4.784940000	1.507420000	0.000110000
8	-5.944800000	1.164960000	0.000130000
1	-4.502840000	2.581680000	0.000600000

## 72

7	4.643990000	0.857090000	-0.000060000
8	5.720790000	0.279620000	0.000070000
8	4.475220000	2.077100000	-0.000330000
32	-1.491560000	-1.482770000	0.000050000
6	3.457240000	0.045320000	0.000050000
6	3.319020000	-1.333630000	0.000300000
6	1.941850000	-1.580280000	0.000290000
6	1.266680000	-0.342320000	0.000010000
7	2.240620000	0.639970000	-0.000090000
6	-0.130970000	-0.029990000	-0.000110000
6	-0.618410000	1.243540000	-0.000340000
6	-2.046180000	1.422230000	-0.001060000
7	-2.546530000	2.910160000	0.000050000
1	4.125470000	-2.047490000	0.000470000
1	1.457730000	-2.542340000	0.000460000
1	2.128040000	1.644240000	-0.000290000
1	-0.003170000	2.132140000	-0.000250000
8	-2.881050000	0.558530000	-0.000740000
8	-1.677320000	3.770040000	0.000650000
8	-3.742100000	3.072960000	0.000610000
9	-2.401560000	-1.679620000	-1.462130000
9	-0.602110000	-2.996670000	-0.000050000
9	-2.401260000	-1.679680000	1.462410000

## 73

16	-2.631870000	-1.837360000	0.611550000
8	-2.043380000	-3.168160000	0.559810000
6	-3.782320000	-1.839630000	-0.749550000
7	-4.491020000	-2.014790000	-1.643540000
8	-3.299010000	-1.372310000	1.808960000
6	2.184310000	-0.578500000	0.095600000
6	1.984050000	-1.981420000	0.175220000
6	0.618880000	-2.211760000	0.201420000
6	-0.058580000	-0.972710000	0.128890000
7	0.952410000	0.004650000	0.040650000
6	-1.410880000	-0.585590000	0.073160000
6	-1.818690000	0.696850000	-0.255160000
6	-3.126370000	1.249290000	-0.205200000
7	-3.086750000	2.839130000	-0.596140000
1	2.757730000	-2.730090000	0.189660000

1	0.133130000	-3.170530000	0.234850000
1	0.781310000	0.988940000	0.163000000
1	-1.066790000	1.386560000	-0.608420000
8	-4.209870000	0.818580000	0.044990000
8	-1.994040000	3.372880000	-0.770000000
8	-4.161570000	3.383900000	-0.673810000
7	3.332770000	0.127030000	0.071170000
6	4.623970000	-0.563760000	0.170470000
6	3.337220000	1.584200000	-0.093850000
6	5.195680000	-1.004020000	-1.183600000
1	5.319590000	0.118540000	0.667330000
1	4.263290000	1.849120000	-0.610780000
1	2.527320000	1.869930000	-0.773320000
6	3.240420000	2.365390000	1.225570000
1	4.068330000	2.064440000	1.875950000
6	3.273780000	3.879160000	0.998880000
1	2.322500000	2.086600000	1.754300000
1	3.210610000	4.415270000	1.948000000
1	4.200140000	4.187420000	0.504840000
1	2.437310000	4.210580000	0.376670000
1	4.511660000	-1.423200000	0.835730000
6	6.550630000	-1.700990000	-1.033510000
1	4.480450000	-1.672130000	-1.673310000
1	5.297220000	-0.128300000	-1.833490000
1	6.942410000	-2.004950000	-2.006530000
1	7.290690000	-1.041450000	-0.570030000
1	6.471390000	-2.599300000	-0.413850000

#### 74

16	-1.464550000	-1.875230000	0.416420000
8	-0.755910000	-3.115930000	0.138350000
6	-2.697400000	-1.802730000	-0.867550000
7	-3.446670000	-1.917690000	-1.737860000
8	-2.090220000	-1.654320000	1.702680000
6	3.169400000	-0.075510000	-0.143610000
6	3.107000000	-1.482410000	-0.290410000
6	1.771120000	-1.850900000	-0.239940000
6	0.981810000	-0.692300000	-0.067280000
7	1.890640000	0.382130000	-0.030180000
6	-0.403660000	-0.439400000	0.006820000
6	-0.946580000	0.827400000	-0.103370000
6	-2.295990000	1.233240000	0.096420000
7	-2.432070000	2.855960000	-0.054300000
1	3.946570000	-2.144060000	-0.418070000
1	1.378650000	-2.846990000	-0.340230000
1	1.637530000	1.315370000	0.250070000
1	-0.286590000	1.633180000	-0.388670000
8	-3.313540000	0.660660000	0.334760000
8	-1.407930000	3.515670000	-0.208520000
8	-3.555660000	3.292820000	0.010500000
7	4.243570000	0.747400000	-0.125330000
6	5.580520000	0.168770000	-0.025570000
6	4.073390000	2.161800000	0.186640000
1	6.309950000	0.912160000	-0.345770000

1	5.819030000	-0.144540000	0.997920000
1	5.667260000	-0.692150000	-0.688130000
1	5.004030000	2.684290000	-0.028180000
1	3.297520000	2.602910000	-0.444490000
1	3.818910000	2.329910000	1.241470000

**75**

16	0.360740000	-1.922720000	-0.405890000
8	-0.684130000	-2.896730000	-0.129830000
6	1.543210000	-2.196620000	0.897210000
7	2.216590000	-2.511450000	1.780050000
8	1.039560000	-1.905040000	-1.683480000
6	-3.558200000	1.139840000	0.084600000
6	-3.906560000	-0.206720000	0.283520000
6	-2.731250000	-0.949850000	0.245440000
6	-1.645940000	-0.073510000	0.036620000
7	-2.208940000	1.215650000	-0.037350000
6	-0.242150000	-0.232390000	-0.021570000
6	0.639980000	0.821650000	0.086460000
6	2.055060000	0.816040000	-0.098470000
7	2.656370000	2.327990000	0.034120000
1	-4.906240000	-0.579120000	0.440740000
1	-2.640440000	-2.012020000	0.386030000
1	-1.711330000	2.030480000	-0.362170000
1	0.238010000	1.787730000	0.354390000
8	2.860510000	-0.033840000	-0.313440000
8	1.865030000	3.257860000	0.158540000
8	3.859100000	2.416240000	-0.012650000
7	-4.361390000	2.231840000	-0.046520000
1	-5.333430000	2.120620000	0.194040000
1	-3.982330000	3.149090000	0.133130000

**76**

16	0.333090000	-1.912230000	-0.419010000
8	-0.731850000	-2.868640000	-0.163130000
6	1.498290000	-2.220440000	0.890710000
7	2.159220000	-2.552770000	1.776630000
8	1.021330000	-1.887550000	-1.691010000
8	-4.254780000	2.307250000	-0.023100000
6	-3.547890000	1.177190000	0.083800000
6	-3.917180000	-0.149350000	0.307720000
6	-2.739500000	-0.901840000	0.276340000
6	-1.654980000	-0.034890000	0.044290000
7	-2.207690000	1.251750000	-0.053950000
6	-0.246250000	-0.211680000	-0.019560000
6	0.645250000	0.825880000	0.093030000
6	2.067710000	0.795190000	-0.084960000
7	2.699660000	2.289310000	0.037260000
1	-4.918740000	-0.513310000	0.473070000
1	-2.655480000	-1.962800000	0.428450000
1	-1.720930000	2.091610000	-0.329390000
1	0.258000000	1.799650000	0.356600000
8	2.850610000	-0.076430000	-0.287380000
8	1.924700000	3.233320000	0.143990000

8	3.904230000	2.349320000	0.001270000
1	-5.197380000	2.123950000	0.062320000

**77**

16	0.501920000	1.694900000	-0.446240000
8	1.829050000	2.247430000	-0.238820000
6	-0.462600000	2.387070000	0.879720000
7	-0.961540000	2.919740000	1.773780000
8	-0.196870000	1.871270000	-1.700700000
1	3.498310000	-3.506290000	-0.087560000
6	3.198450000	-2.478590000	0.044170000
6	3.948050000	-1.354390000	0.362720000
6	3.079380000	-0.254780000	0.360720000
6	1.790090000	-0.722410000	0.050950000
7	1.907420000	-2.099600000	-0.123730000
6	0.504850000	-0.097620000	-0.014520000
6	-0.664130000	-0.791830000	0.120360000
6	-2.010870000	-0.309410000	-0.053320000
7	-3.081610000	-1.525330000	0.046370000
1	5.005810000	-1.339630000	0.570040000
1	3.330640000	0.767960000	0.577230000
1	1.170640000	-2.705230000	-0.450870000
1	-0.603110000	-1.834370000	0.399230000
8	-2.471200000	0.768960000	-0.236530000
8	-2.641120000	-2.668010000	0.094240000
8	-4.242620000	-1.198730000	0.050830000

**78**

16	1.017080000	-1.887030000	-0.450840000
8	0.164380000	-3.043320000	-0.235350000
6	2.214480000	-1.987580000	0.860850000
7	2.926880000	-2.193730000	1.745190000
8	1.691040000	-1.677270000	-1.713230000
17	-4.691720000	1.439730000	-0.055760000
6	-3.431360000	0.290700000	0.108800000
6	-3.502830000	-1.064950000	0.392780000
6	-2.189030000	-1.550400000	0.365990000
6	-1.325360000	-0.480850000	0.074640000
7	-2.135340000	0.648040000	-0.063440000
6	0.096680000	-0.353330000	-0.004610000
6	0.742590000	0.843870000	0.127060000
6	2.144760000	1.120240000	-0.057330000
7	2.444580000	2.710300000	0.050380000
1	-4.404100000	-1.619820000	0.593390000
1	-1.877630000	-2.561840000	0.556400000
1	-1.835140000	1.556510000	-0.383910000
1	0.158480000	1.707270000	0.413210000
8	3.089180000	0.428570000	-0.254270000
8	1.482480000	3.466490000	0.116030000
8	3.609400000	3.022590000	0.042860000

**79**

16	-0.914890000	-1.876350000	0.480350000
8	0.011690000	-2.982370000	0.322320000



6	-2.079080000	-2.088600000	-0.846310000
7	-2.766980000	-2.353260000	-1.734470000
8	-1.625820000	-1.656300000	1.720480000
6	4.478350000	1.516170000	0.122210000
6	3.443480000	0.497090000	-0.069190000
6	3.551950000	-0.846080000	-0.431570000
6	2.266920000	-1.390370000	-0.432040000
6	1.364130000	-0.365800000	-0.083800000
7	2.116730000	0.774590000	0.118830000
6	-0.071360000	-0.308280000	-0.004740000
6	-0.764890000	0.852600000	-0.163060000
6	-2.186070000	1.070710000	0.011680000
7	-2.548370000	2.644670000	-0.058690000
1	4.477610000	-1.348040000	-0.662600000
1	1.991790000	-2.401910000	-0.672370000
1	1.759550000	1.647730000	0.479220000
1	-0.216030000	1.734840000	-0.462760000
8	-3.097330000	0.331360000	0.178170000
8	-1.613120000	3.436090000	-0.053890000
8	-3.723630000	2.909940000	-0.091730000
8	5.659380000	1.309490000	-0.037110000
1	4.105810000	2.516660000	0.428140000

## 80

16	-1.320530000	-1.850090000	0.515460000
8	-0.504660000	-3.042990000	0.382250000
6	-2.504900000	-1.979070000	-0.802570000
7	-3.218750000	-2.193710000	-1.683760000
8	-1.998140000	-1.528290000	1.751260000
7	4.344870000	0.903770000	0.045410000
6	3.236810000	0.008610000	-0.141110000
6	3.218550000	-1.328800000	-0.498740000
6	1.873200000	-1.718420000	-0.475860000
6	1.099600000	-0.600330000	-0.114650000
7	1.973560000	0.451250000	0.077170000
6	-0.325170000	-0.386240000	-0.013890000
6	-0.888480000	0.836870000	-0.187940000
6	-2.285040000	1.202240000	-0.013590000
7	-2.492200000	2.797710000	-0.097970000
1	4.080170000	-1.928070000	-0.740840000
1	1.484020000	-2.693610000	-0.708270000
1	1.770790000	1.376830000	0.431940000
1	-0.251280000	1.653370000	-0.500820000
8	-3.259890000	0.552170000	0.159510000
8	-1.482390000	3.489530000	-0.103090000
8	-3.636250000	3.175340000	-0.131530000
8	5.464470000	0.465900000	-0.174290000
8	4.072500000	2.047160000	0.412750000

## 81

7	-2.708120000	0.087830000	-0.327590000
6	-2.571310000	1.549440000	-0.104590000
6	-3.747670000	2.396490000	-0.593870000

6	-3.439590000	3.889210000	-0.429610000
6	-4.047820000	-0.539510000	-0.297700000
6	-4.571200000	-0.775840000	1.125040000
6	-5.964580000	-1.410850000	1.112820000
1	-2.401360000	1.729440000	0.964580000
1	-1.681030000	1.880140000	-0.647440000
1	-3.945910000	2.172990000	-1.646660000
1	-4.652560000	2.152740000	-0.031610000
1	-4.286230000	4.489180000	-0.766560000
1	-3.247630000	4.147120000	0.615540000
1	-2.568210000	4.187870000	-1.018880000
1	-4.723890000	0.106790000	-0.855210000
1	-3.995400000	-1.476790000	-0.851420000
1	-3.867820000	-1.419930000	1.663600000
1	-4.601440000	0.176160000	1.664860000
1	-6.319150000	-1.576060000	2.131670000
1	-6.692920000	-0.769550000	0.609030000
1	-5.959850000	-2.378350000	0.602770000
6	-1.622690000	-0.682970000	-0.343300000
6	-1.505430000	-2.103040000	-0.515680000
6	-0.170360000	-2.423970000	-0.470960000
6	0.572110000	-1.233530000	-0.265250000
7	-0.344760000	-0.194150000	-0.196770000
6	1.956120000	-1.004450000	-0.145510000
6	2.672940000	0.175830000	0.022210000
6	4.090620000	0.201070000	0.161240000
7	4.655810000	1.676580000	0.343300000
1	-2.320680000	-2.790220000	-0.661430000
1	0.242220000	-3.415140000	-0.583450000
1	-0.113960000	0.761420000	0.022600000
7	2.685010000	-2.200430000	-0.206700000
1	2.139890000	1.113460000	0.048850000
8	4.879550000	-0.702170000	0.159400000
8	3.830580000	2.582010000	0.359780000
8	5.851020000	1.772910000	0.450890000
7	3.226330000	-3.161340000	-0.262290000

## 82

6	2.840220000	0.010780000	-0.000050000
6	2.941590000	1.438970000	-0.000090000
6	1.663890000	1.947670000	-0.000070000
6	0.747150000	0.867010000	-0.000020000
7	1.501760000	-0.299300000	-0.000010000
6	-0.661030000	0.837050000	-0.000010000
6	-1.552400000	-0.228090000	-0.000030000
6	-2.968310000	-0.048950000	0.000050000
7	-3.754440000	-1.430550000	-0.000040000
7	3.787850000	-0.923950000	-0.000080000
1	3.853770000	2.010230000	-0.000100000
1	1.406550000	2.995980000	-0.000100000
1	1.123980000	-1.233660000	0.000090000
7	-1.205070000	2.132210000	0.000040000
1	-1.166980000	-1.235930000	-0.000110000
8	-3.612760000	0.961500000	0.000100000

6	3.431740000	-2.346970000	0.000140000
6	5.216060000	-0.587140000	0.000030000
1	4.346200000	-2.935180000	-0.000080000
1	2.861090000	-2.607880000	0.896820000
1	2.860590000	-2.608010000	-0.896190000
1	5.690670000	-1.004200000	0.890870000
1	5.691030000	-1.005540000	-0.889980000
1	5.357510000	0.489260000	-0.000790000
8	-3.071880000	-2.447800000	-0.000040000
8	-4.955370000	-1.352120000	-0.000050000
7	-1.595500000	3.164520000	0.000080000

### 83

7	4.194990000	-1.919010000	-0.000060000
6	3.398340000	-0.847000000	0.000010000
6	3.758670000	0.527770000	0.000130000
6	2.589660000	1.258940000	0.000130000
6	1.497320000	0.358300000	-0.000020000
7	2.036160000	-0.926080000	-0.000100000
6	0.104900000	0.580280000	-0.000040000
6	-0.966700000	-0.295300000	-0.000100000
6	-2.330470000	0.145640000	-0.000210000
7	-3.360570000	-1.062070000	0.000080000
1	4.767970000	0.907190000	0.000210000
1	2.522810000	2.336340000	0.000200000
1	1.504780000	-1.784310000	-0.000150000
7	-0.197600000	1.959650000	-0.000030000
1	-0.777940000	-1.358220000	-0.000060000
8	-2.768410000	1.259380000	-0.000050000
8	-4.524570000	-0.758900000	0.000140000
8	-2.876420000	-2.186590000	0.000050000
7	-0.388880000	3.045110000	-0.000010000
1	5.196940000	-1.803000000	0.000110000
1	3.841670000	-2.863920000	-0.000050000

### 84

6	3.401040000	-0.856010000	0.000070000
6	3.774150000	0.501420000	0.000300000
6	2.596980000	1.235200000	0.000220000
6	1.509690000	0.332790000	-0.000050000
7	2.048230000	-0.947450000	-0.000140000
6	0.112910000	0.559100000	-0.000190000
6	-0.960540000	-0.302310000	-0.000400000
6	-2.330150000	0.150940000	-0.000560000
7	-3.370920000	-1.043730000	0.000140000
1	4.783030000	0.882320000	0.000500000
1	2.530630000	2.312660000	0.000360000
1	1.550430000	-1.827420000	-0.000340000
1	-0.780990000	-1.367630000	-0.000430000
8	-2.749230000	1.269200000	0.000060000
8	-2.893140000	-2.169780000	-0.000130000
8	-4.530470000	-0.726800000	0.000620000
7	-0.186780000	1.946750000	-0.000120000
7	-0.363730000	3.033330000	-0.000050000

8	4.092540000	-1.976140000	0.000010000
1	5.047260000	-1.820780000	0.000170000

**85**

6	3.575200000	-1.529060000	-0.000050000
6	4.119170000	-0.244610000	0.000120000
6	3.056060000	0.655840000	0.000150000
6	1.861850000	-0.095590000	0.000000000
7	2.222990000	-1.431630000	-0.000120000
6	0.503380000	0.323120000	0.000020000
6	-0.676990000	-0.370700000	0.000070000
6	-1.978730000	0.271980000	-0.000010000
7	-3.174710000	-0.765600000	0.000000000
1	5.170590000	-0.006750000	0.000210000
1	3.136120000	1.732340000	0.000290000
1	1.596390000	-2.223680000	-0.000280000
1	-0.652950000	-1.451280000	0.000170000
8	-2.231240000	1.436500000	-0.000090000
8	-2.852920000	-1.945350000	-0.000110000
8	-4.277650000	-0.290060000	0.000210000
7	0.397970000	1.746290000	-0.000070000
7	0.385410000	2.846180000	-0.000130000
1	4.062950000	-2.491930000	-0.000150000

**86**

6	3.145160000	-0.312620000	0.000000000
6	3.352260000	1.070700000	0.000310000
6	2.095480000	1.664770000	0.000290000
6	1.126540000	0.638830000	0.000050000
7	1.809160000	-0.566120000	-0.000050000
6	-0.292510000	0.701680000	0.000070000
6	-1.257340000	-0.273510000	0.000180000
6	-2.676620000	0.017790000	0.000020000
7	-3.570960000	-1.288450000	0.000070000
17	4.281690000	-1.566620000	-0.000190000
1	4.312860000	1.559210000	0.000490000
1	1.903020000	2.727090000	0.000500000
1	1.411570000	-1.495420000	-0.000400000
1	-0.958310000	-1.312140000	0.000410000
8	-3.217030000	1.080830000	-0.000270000
8	-2.962170000	-2.349200000	0.000140000
8	-4.758660000	-1.107880000	0.000010000
7	-0.751990000	2.048180000	-0.000120000
7	-1.045170000	3.108940000	-0.000230000

**87**

6	3.157190000	-0.453060000	0.000000000
6	3.385530000	0.928170000	0.000210000
6	2.145630000	1.555600000	0.000220000
6	1.156810000	0.546130000	0.000040000
7	1.808550000	-0.667240000	-0.000100000
6	-0.265410000	0.647710000	0.000040000
6	-1.253610000	-0.297560000	0.000120000
6	-2.672050000	0.028250000	0.000000000

7	-3.596570000	-1.255740000	0.000050000
1	4.360070000	1.390090000	0.000330000
1	1.973240000	2.621450000	0.000380000
1	1.377690000	-1.581960000	-0.000330000
1	-0.983220000	-1.344360000	0.000280000
8	-3.181680000	1.104330000	-0.000140000
8	-3.009490000	-2.328460000	-0.000110000
8	-4.778810000	-1.046980000	0.000200000
7	-0.691790000	2.008760000	-0.000120000
7	-0.955420000	3.076830000	-0.000230000
6	4.140090000	-1.563310000	-0.000130000
8	5.324150000	-1.352240000	-0.000040000
1	3.720350000	-2.588030000	-0.000290000

## 88

6	2.922930000	-0.048250000	0.000010000
6	3.079940000	1.329550000	0.000050000
6	1.787120000	1.859600000	-0.000030000
6	0.877880000	0.781460000	-0.000010000
7	1.611230000	-0.382320000	-0.000050000
6	-0.553040000	0.775530000	0.000040000
6	-1.459620000	-0.242940000	0.000320000
6	-2.906130000	-0.029180000	0.000240000
7	-3.728320000	-1.378660000	0.000190000
7	3.918410000	-1.108650000	-0.000010000
1	4.018710000	1.859230000	0.000110000
1	1.539360000	2.910390000	-0.000020000
1	1.302890000	-1.348750000	-0.000140000
7	-1.083920000	2.100270000	-0.000400000
1	-1.106900000	-1.265750000	0.000570000
8	-3.490850000	1.006340000	0.000200000
8	3.474720000	-2.251470000	-0.000060000
8	5.082630000	-0.763480000	0.000020000
8	-3.057230000	-2.400100000	-0.001670000
8	-4.922550000	-1.260120000	0.001810000
7	-1.423470000	3.146610000	-0.000670000

## 89

C	-2.73817	-0.75382	0.00006
C	-2.93038	0.61657	0.00046
C	-1.65273	1.21509	-0.00035
C	-0.69618	0.19964	-0.00003
N	-1.39491	-0.99612	-0.00047
C	0.72741	0.31270	0.00014
C	1.64659	-0.68301	0.00028
C	3.08324	-0.39814	0.00034
O	3.58192	0.71274	-0.00026
H	-3.45197	-1.56207	0.00013
H	-3.88506	1.11790	0.00093
H	-1.42869	2.27080	-0.00047
H	-0.97440	-1.91071	-0.00104
H	1.11070	1.32967	0.00002
H	1.36452	-1.73258	0.00037

H	3.73521	-1.29633	0.00010
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**90**

6	4.928330000	0.687260000	0.440450000
6	5.398490000	-0.567030000	0.103650000
6	4.271170000	-1.371010000	-0.186030000
6	3.128420000	-0.593750000	-0.021280000
7	3.562070000	0.662990000	0.362630000
6	1.754680000	-0.970330000	-0.200870000
6	0.657100000	-0.202860000	-0.045560000
6	-0.685650000	-0.787110000	-0.301000000
8	-0.812010000	-1.947310000	-0.693140000
1	6.434990000	-0.863260000	0.071760000
1	4.271420000	-2.407840000	-0.485580000
1	2.961430000	1.446060000	0.558520000
1	1.588630000	-2.000490000	-0.502010000
1	0.741940000	0.837830000	0.241870000
1	5.455810000	1.583220000	0.726130000
7	-1.789190000	0.013060000	-0.099180000
6	-1.758240000	1.377670000	0.427350000
6	-1.615290000	2.463700000	-0.648900000
6	-1.654940000	3.876430000	-0.060080000
6	-3.105410000	-0.551060000	-0.415620000
6	-3.759320000	-1.277250000	0.767070000
6	-5.137450000	-1.838900000	0.407750000
1	-2.690970000	1.535180000	0.978450000
1	-0.962420000	1.472240000	1.169790000
1	-0.678170000	2.306750000	-1.193130000
1	-2.417950000	2.343160000	-1.384140000
1	-1.552290000	4.633460000	-0.841400000
1	-2.599030000	4.064620000	0.460870000
1	-0.845240000	4.033240000	0.660250000
1	-3.748600000	0.266940000	-0.757750000
1	-2.979440000	-1.247200000	-1.245560000
1	-3.094180000	-2.086120000	1.081410000
1	-3.849090000	-0.588990000	1.615930000
1	-5.586800000	-2.356760000	1.259000000
1	-5.827200000	-1.045300000	0.101440000
1	-5.068150000	-2.555230000	-0.416440000

**91**

C	-3.80576	1.05910	0.04478
C	-4.26948	-0.24139	-0.00062
C	-3.13634	-1.08700	-0.03540
C	-1.99647	-0.28835	-0.01097
N	-2.43797	1.02229	0.03752
C	-0.61941	-0.69185	-0.02982
C	0.47612	0.09468	-0.01128
C	1.82359	-0.53073	-0.01553
O	1.95979	-1.75274	0.01590
H	-4.33935	1.99534	0.08175
H	-5.30561	-0.54057	-0.00750
H	-3.13056	-2.16551	-0.07422

H	-1.84117	1.83174	0.06875
H	-0.44768	-1.76376	-0.06058
H	0.38656	1.17307	0.02911
C	4.24903	-0.26234	0.08321
H	4.88960	0.06024	-0.74401
H	4.71337	0.05154	1.02599
H	4.16282	-1.34559	0.07182
N	2.91608	0.31177	-0.05427
C	2.83996	1.76709	-0.05670
H	3.79440	2.16151	-0.40931
H	2.07124	2.12828	-0.74029
H	2.65386	2.18200	0.94255

## 92

C	3.11011	-0.91390	-0.01091
C	3.43737	0.42820	0.01200
C	2.22342	1.15294	0.01939
C	1.17226	0.24048	0.00159
N	1.74625	-1.01857	-0.01617
C	-0.23848	0.49926	0.00221
C	-1.24999	-0.39104	-0.00298
C	-2.65563	0.07871	-0.00449
O	-2.97645	1.25885	-0.02530
H	3.73768	-1.79058	-0.02453
H	4.43710	0.83246	0.02187
H	2.10651	2.22568	0.03647
H	1.23664	-1.88592	-0.03890
H	-0.52006	1.54870	0.00666
H	-1.07307	-1.46349	-0.00931
N	-3.60088	-0.92086	-0.00514
H	-4.56611	-0.64723	0.09202
H	-3.35904	-1.88240	0.16639

## 93

C	3.58451	-0.97843	0.00579
C	3.95741	0.35140	-0.03306
C	2.76914	1.11736	-0.03599
C	1.68757	0.24158	-0.00021
N	2.21813	-1.03616	0.02447
C	0.28658	0.54814	0.00765
C	-0.75360	-0.30893	0.02527
C	-2.14024	0.20217	0.03950
O	-2.44140	1.38946	0.06235
H	4.18167	-1.87602	0.02258
H	4.97022	0.72103	-0.05597
H	2.68923	2.19330	-0.06226
H	1.67969	-1.88542	0.06129
H	0.04196	1.60663	-0.00084
H	-0.61347	-1.38673	0.03749
N	-3.10845	-0.78111	0.03978
N	-4.47097	-0.46588	-0.11872
H	-2.86613	-1.71670	-0.24920
H	-4.83972	-0.18953	0.78796
H	-4.53141	0.36001	-0.71222

**94**

C	-3.09795	-0.91089	0.00005
C	-3.43087	0.43136	0.00005
C	-2.22096	1.15959	0.00001
C	-1.16612	0.24912	0.00001
N	-1.73583	-1.01218	0.00005
C	0.24122	0.50937	-0.00002
C	1.24755	-0.39087	-0.00001
C	2.64237	0.05627	-0.00004
O	3.03892	1.20203	-0.00006
H	-3.72330	-1.78931	0.00007
H	-4.43217	0.83161	0.00006
H	-2.10777	2.23290	-0.00002
H	-1.22280	-1.87832	0.00006
H	0.51866	1.55970	-0.00004
H	1.08479	-1.46235	0.00001
O	3.50404	-1.00225	-0.00002
H	4.39829	-0.63102	-0.00004

**95**

C	3.32569	1.10496	-0.00014
C	3.81856	-0.18689	0.00022
C	2.70584	-1.05634	0.00024
C	1.54778	-0.28127	-0.00005
N	1.96087	1.04034	-0.00023
C	0.18481	-0.71729	-0.00004
C	-0.93291	0.04291	-0.00002
C	-2.25496	-0.61538	-0.00004
O	-2.41203	-1.81350	-0.00022
H	3.84007	2.05266	-0.00032
H	4.86097	-0.46288	0.00043
H	2.72315	-2.13542	0.00050
H	1.34844	1.83889	-0.00078
H	0.04374	-1.79415	-0.00006
H	-0.87529	1.12379	0.00006
O	-3.37254	0.17151	0.00002
C	-3.30241	1.59842	0.00025
H	-4.33665	1.93891	0.00031
H	-2.80416	1.97838	0.89686
H	-2.80418	1.97867	-0.89625

**96**

C	-3.10605	-0.94353	-0.00021
C	-3.45868	0.39362	-0.00048
C	-2.25956	1.13983	-0.00023
C	-1.19051	0.24568	-0.00012
N	-1.74218	-1.02401	-0.00008
C	0.21265	0.52711	-0.00001
C	1.24150	-0.34977	0.00015
C	2.64352	0.11820	0.00028
O	2.94106	1.30247	0.00020
H	-3.71829	-1.83116	-0.00020
H	-4.46587	0.77894	-0.00071



H	-2.16211	2.21466	-0.00026
H	-1.21572	-1.88178	0.00004
H	0.47521	1.58182	-0.00003
H	1.07892	-1.42438	0.00020
C	3.71146	-0.96122	0.00040
H	4.69965	-0.50375	0.00044
H	3.60447	-1.60271	0.88147
H	3.60459	-1.60281	-0.88060

### 97

C	-4.09522	-1.79619	-0.27992
C	-4.93793	-0.91776	0.37674
C	-4.19786	0.25816	0.62894
C	-2.91228	0.08059	0.12016
N	-2.88148	-1.18842	-0.43212
C	-1.80864	0.99092	0.13479
C	-0.57431	0.81060	-0.38720
C	0.45499	1.86075	-0.28816
O	0.26991	2.92074	0.28944
H	-4.26881	-2.79649	-0.64317
H	-5.96581	-1.10983	0.64032
H	-4.54503	1.15152	1.12506
H	-2.07544	-1.61026	-0.86302
H	-1.99626	1.94094	0.62800
H	-0.29511	-0.10688	-0.89626
C	1.80082	1.56628	-0.96289
H	1.62423	1.41445	-2.03339
H	2.41408	2.46266	-0.84919
C	2.50458	0.35281	-0.38806
C	2.77776	-0.77125	-1.17374
C	3.42596	-1.88256	-0.63416
C	3.81008	-1.88498	0.70462
C	3.54421	-0.76871	1.49825
C	2.89807	0.33910	0.95659
H	2.49016	-0.77404	-2.22067
H	3.63434	-2.74226	-1.26168
H	4.31541	-2.74647	1.12635
H	3.84257	-0.76054	2.54079
H	2.69538	1.20358	1.58046

### 98

C	-3.08133	-0.91197	0.00001
C	-3.41982	0.43029	0.00015
C	-2.21451	1.16179	0.00009
C	-1.15514	0.25391	0.00003
N	-1.72091	-1.01014	0.00006
C	0.24645	0.52188	-0.00001
C	1.26093	-0.37491	-0.00004
C	2.64031	0.08339	-0.00007
O	3.08429	1.18826	-0.00009
H	-3.70468	-1.79188	-0.00002
H	-4.42266	0.82634	0.00022
H	-2.10486	2.23547	0.00012
H	-1.20692	-1.87591	0.00005

H	0.51429	1.57459	-0.00001
H	1.10684	-1.44670	-0.00003
F	3.50319	-0.99370	-0.00012

**99**

C	-3.44551	-1.05723	0.00001
C	-3.88680	0.25390	-0.00015
C	-2.74116	1.07769	-0.00013
C	-1.61448	0.25611	0.00006
N	-2.08019	-1.04804	0.00015
C	-0.23689	0.63571	0.00007
C	0.85118	-0.16892	0.00001
C	2.19533	0.42568	0.00009
O	2.43410	1.61099	0.00014
H	-3.99780	-1.98334	0.00006
H	-4.91737	0.57113	-0.00030
H	-2.71542	2.15659	-0.00028
H	-1.50058	-1.87085	0.00064
H	-0.05320	1.70635	0.00015
H	0.76981	-1.24952	-0.00011
S	3.61552	-0.72125	-0.00013
H	2.92463	-1.87957	-0.00002

**100**

C	-3.40798	-1.07519	-0.00012
C	-3.87479	0.22864	0.00008
C	-2.74645	1.07276	-0.00010
C	-1.60371	0.27090	0.00001
N	-2.04517	-1.04215	0.00005
C	-0.23606	0.67298	0.00004
C	0.85945	-0.12682	0.00010
C	2.18653	0.46725	0.00012
O	2.50121	1.61486	-0.00005
H	-3.94384	-2.01097	-0.00017
H	-4.91125	0.52573	0.00016
H	-2.74092	2.15198	-0.00015
H	-1.45032	-1.85460	0.00013
H	-0.07198	1.74651	0.00001
H	0.80500	-1.20680	0.00013
Cl	3.50340	-0.82581	-0.00005

**101**

C	-3.70767	1.07714	0.00009
C	-4.19818	-0.21859	0.00003
C	-3.08504	-1.08288	-0.00003
C	-1.92750	-0.30152	-0.00000
N	-2.34605	1.01877	0.00004
C	-0.56434	-0.71847	-0.00003
C	0.53746	0.07327	-0.00002
C	1.87127	-0.50262	-0.00005
O	2.13610	-1.69902	-0.00011
H	-4.22657	2.02244	0.00015
H	-5.24002	-0.49660	0.00003
H	-3.09849	-2.16203	-0.00008

H	-1.73266	1.81776	0.00006
H	-0.40556	-1.79367	-0.00007
H	0.49035	1.15532	0.00001
C	3.03328	0.52630	-0.00009
O	2.83588	1.73112	-0.00020
N	4.24660	-0.06690	0.00027
H	5.08139	0.49605	0.00038
H	4.29620	-1.07495	0.00046

**102**

C	-3.26843	1.09344	-0.00008
C	-3.76338	-0.20072	0.00014
C	-2.65368	-1.06857	0.00019
C	-1.49307	-0.29132	0.00001
N	-1.90713	1.03075	-0.00017
C	-0.13326	-0.71654	-0.00002
C	0.97779	0.06274	-0.00022
C	2.30766	-0.52612	-0.00024
O	2.57316	-1.72126	0.00035
H	-3.78436	2.04037	-0.00019
H	-4.80614	-0.47505	0.00025
H	-2.67071	-2.14765	0.00035
H	-1.29246	1.82858	-0.00032
H	0.01681	-1.79300	0.00013
H	0.93666	1.14624	-0.00038
C	3.49338	0.44994	0.00006
O	3.38607	1.65049	-0.00013
H	4.47417	-0.06571	0.00058

**103**

C	-4.63602	-1.09974	-0.00003
C	-5.19821	0.16581	-0.00009
C	-4.13527	1.09144	-0.00002
C	-2.93599	0.37707	0.00007
N	-3.27906	-0.96509	0.00005
C	-1.60124	0.87874	0.00013
C	-0.44991	0.16337	0.00012
C	0.83684	0.85337	0.00019
O	0.99080	2.05255	0.00013
H	-5.10070	-2.07285	-0.00004
H	-6.25392	0.38513	-0.00017
H	-4.20959	2.16814	-0.00006
H	-2.62511	-1.73078	0.00023
H	-1.51249	1.96133	0.00019
H	-0.44698	-0.91904	0.00005
C	2.10985	-0.08125	-0.00002
Cl	2.05699	-1.12878	-1.47462
Cl	3.60491	0.87181	-0.00059
Cl	2.05783	-1.12829	1.47499

**104**

C	-3.98674	-1.12924	-0.00002
C	-4.51763	0.15057	-0.00002
C	-3.43281	1.04862	0.00000

C	-2.25078	0.30412	0.00001
N	-2.62777	-1.02944	-0.00001
C	-0.90632	0.77223	0.00003
C	0.23224	0.03310	0.00005
C	1.53415	0.68538	0.00007
O	1.74785	1.87953	-0.00004
H	-4.47627	-2.09011	-0.00003
H	-5.56759	0.39577	-0.00003
H	-3.47992	2.12683	0.00001
H	-1.99370	-1.81179	-0.00000
H	-0.79160	1.85267	0.00004
H	0.21804	-1.05090	0.00005
C	2.74746	-0.29268	-0.00000
F	2.70870	-1.09968	1.08960
F	2.70840	-1.09991	-1.08943
F	3.91458	0.34567	-0.00023

### 105

1	5.443580000	2.140270000	-0.000050000
6	4.999020000	1.157760000	-0.000030000
6	5.589690000	-0.096440000	-0.000010000
6	4.548710000	-1.043690000	0.000010000
6	3.332120000	-0.355020000	0.000020000
7	3.646930000	0.994990000	0.000000000
6	2.012100000	-0.883520000	0.000050000
6	0.838310000	-0.195710000	0.000060000
6	-0.435700000	-0.901970000	0.000090000
1	6.650010000	-0.291890000	-0.000020000
1	4.645810000	-2.118550000	0.000020000
1	2.976560000	1.746570000	0.000000000
1	0.806050000	0.888040000	0.000040000
8	-0.568480000	-2.118510000	-0.000020000
1	1.945170000	-1.968160000	0.000060000
14	-2.102150000	0.084730000	0.000000000
17	-1.815540000	2.142670000	-0.000600000
17	-3.190180000	-0.415560000	-1.672070000
17	-3.189770000	-0.414620000	1.672620000

### 106

C	-3.27041	-1.09102	-0.00026
C	-3.73195	0.21619	-0.00001
C	-2.60118	1.05394	-0.00011
C	-1.46008	0.24625	0.00002
N	-1.90884	-1.06540	0.00038
C	-0.09465	0.64267	0.00004
C	1.00576	-0.15490	0.00031
C	2.34046	0.42698	0.00035
O	2.61463	1.61440	-0.00038
H	-3.81169	-2.02378	-0.00039
H	-4.76720	0.51736	-0.00003
H	-2.58984	2.13311	-0.00020
H	-1.31851	-1.88127	0.00071
H	0.07741	1.71538	-0.00012
H	0.94419	-1.23787	0.00052

C	3.44188	-0.56571	-0.00002
N	4.30450	-1.33238	-0.00030

**107**

6	4.827480000	1.159020000	-0.000600000
6	5.394090000	-0.108060000	-0.000070000
6	4.335980000	-1.032960000	0.000500000
6	3.132330000	-0.318510000	0.000240000
7	3.474330000	1.025450000	-0.000510000
6	1.804690000	-0.817920000	0.000610000
6	0.650830000	-0.092580000	0.000350000
6	-0.632030000	-0.759040000	0.000780000
8	-0.879790000	-1.940930000	0.000960000
1	6.450360000	-0.324060000	-0.000050000
1	4.411250000	-2.109580000	0.001030000
1	2.819650000	1.791530000	-0.000900000
1	1.714450000	-1.900590000	0.001150000
1	0.636140000	0.990520000	-0.000190000
1	5.292680000	2.132000000	-0.001100000
15	-2.097960000	0.492950000	-0.000310000
17	-3.245530000	-0.095680000	-1.615050000
17	-3.245850000	-0.093370000	1.615060000
8	-1.733000000	1.926170000	-0.001280000

**108**

1	4.854750000	-2.037600000	0.000020000
6	4.379170000	-1.069640000	0.000000000
6	4.932250000	0.203170000	-0.000270000
6	3.864730000	1.116490000	0.000040000
6	2.668470000	0.389650000	-0.000030000
7	3.024650000	-0.951030000	0.000050000
6	1.339350000	0.883390000	-0.000030000
6	0.182610000	0.163800000	0.000010000
6	-1.091250000	0.843380000	0.000030000
1	5.986080000	0.430390000	-0.000480000
1	3.928810000	2.193840000	0.000060000
1	2.381510000	-1.726430000	0.000140000
1	0.178720000	-0.919480000	0.000030000
8	-1.319430000	2.022990000	-0.000030000
1	1.248520000	1.965750000	-0.000040000
6	-3.628930000	0.599580000	-0.000170000
7	-4.604450000	1.209530000	-0.000580000
6	-2.308840000	-1.023110000	1.205980000
7	-2.200660000	-1.663240000	2.157690000
6	-2.387850000	-0.184600000	0.000030000
6	-2.308640000	-1.023450000	-1.205680000
7	-2.200860000	-1.664180000	-2.157010000

**109**

1	5.064220000	-2.284210000	0.000180000
6	4.666690000	-1.281640000	0.000090000
6	5.319190000	-0.056360000	0.000230000
6	4.327670000	0.938690000	-0.000190000
6	3.077150000	0.308650000	-0.000020000

7	3.326180000	-1.056010000	-0.000180000
6	1.789460000	0.900960000	0.000000000
6	0.583100000	0.263500000	-0.000070000
6	-0.651930000	1.015680000	-0.000080000
1	6.387780000	0.086370000	0.000450000
1	4.476840000	2.007570000	-0.000300000
1	2.621900000	-1.776550000	-0.000270000
1	0.493850000	-0.816950000	-0.000120000
8	-0.813550000	2.212050000	0.000060000
1	1.777760000	1.987120000	0.000010000
32	-2.324100000	-0.173600000	0.000010000
9	-3.377540000	0.026610000	-1.380950000
9	-1.899920000	-1.885390000	0.000000000
9	-3.377430000	0.026630000	1.381040000

### 110

6	4.368840000	-1.243260000	-0.248530000
6	5.012130000	-0.084710000	0.168150000
6	4.020270000	0.887850000	0.367890000
6	2.778330000	0.311410000	0.070540000
7	3.033980000	-0.999750000	-0.304390000
6	1.494520000	0.904380000	0.128440000
6	0.300780000	0.309070000	-0.163250000
6	-0.911010000	1.060340000	-0.055350000
8	-1.183910000	2.179100000	0.225770000
1	6.075210000	0.028240000	0.306920000
1	4.162730000	1.906860000	0.693630000
1	2.337820000	-1.673710000	-0.581750000
1	1.479350000	1.944600000	0.440350000
1	0.213610000	-0.719810000	-0.483740000
1	4.771090000	-2.210560000	-0.505030000
16	-2.475290000	-0.112920000	-0.517490000
8	-3.635720000	0.695440000	-0.845250000
8	-2.054200000	-1.221260000	-1.372600000
17	-2.827390000	-0.974560000	1.462910000

### 111

6	-4.487490000	-1.084790000	-0.252250000
6	-5.037250000	0.179210000	-0.080460000
6	-3.968700000	1.074250000	0.082770000
6	-2.774130000	0.345610000	0.009030000
7	-3.134540000	-0.978370000	-0.197210000
6	-1.445290000	0.820680000	0.115400000
6	-0.295710000	0.087160000	0.044480000
6	0.976400000	0.733510000	0.168960000
8	1.312940000	1.875010000	0.275770000
1	-6.090070000	0.410920000	-0.076160000
1	-4.029390000	2.140380000	0.239300000
1	-2.493160000	-1.749270000	-0.296480000
1	-1.348270000	1.891410000	0.270140000
1	-0.287100000	-0.983550000	-0.116340000
1	-4.966680000	-2.038390000	-0.408170000
16	2.417140000	-0.589670000	0.199960000

8	2.846090000	-0.845530000	1.570640000
8	2.129680000	-1.693610000	-0.715590000
6	3.719960000	0.385840000	-0.564910000
7	4.577970000	0.953740000	-1.087990000