

ENSDF analysis and utility codes II E0 transitions extension of BrIcc BrIccEmis

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ICTP-IAEA ENSDF workshop, Trieste, August 2016





EO transitions

- $\Box \ \mathbf{J}^{\pi} \rightarrow \mathbf{J}^{\pi}$
- □ No transfer of angular momentum
- □ No change in parity
- Single photon emission is not allowed
- □ For J≠0 E0 can be mixed with E2+M1
- Internal conversion electron emission
- □ Internal pair emission (E>1.022 MeV)
- Double photon emission (E1+E1; ~10⁻⁴ 1964Al18)

$$0^+ \xrightarrow{E1} 1^- \xrightarrow{E1} 0^+$$





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BrIcc v2.3S

THE AUSTRALIAN NATIONAL UNIVERSITY



BrIccS v2.3 (9-Dec-2011) Z=26 (Fe, Iron) γ-energy: 2561 keV Data Sets: PaOmg		
Shell	E(ce)	Ω(E0)
К	2553.89	2.461E+08
IPF		4.151E+09
Tot		4.397E+09
K/Tot		5.597E-02



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$$\frac{\text{Absolute EO transition rate}}{\lambda(E0)} = \frac{1}{\tau_{E0}} = \lambda_{CE}(E0) + \lambda_{CE}(E0)$$
$$= \rho^{2}(E0) \times [\Omega_{CE} + \Omega_{PF}]$$

<u>Monopole matrix element</u> (R=r_oA^{1/3}) $\rho(E0) \frac{\langle f | M(E0) | i \rangle}{eR^2}$

Reduced EO transition probability B(E0)= $\rho^2(E0) \times e^2 R^4$







$$\frac{\text{Absolute EO transition rate}}{\lambda(E0) = \frac{1}{\tau_{E0}} = \lambda_{CE}(E0) + \lambda_{CE}(E0)}$$
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Monopole matrix element (R=r_oA^{1/3})

 $\rho(E0)\frac{\langle f|M(E0)|i\rangle}{eR^2}$

Reduced EO transition probability $B(E0) = \rho^2(E0) \times e^2 R^4$ How to extract $\rho(E0)$ and B(E0)?

<u>EO/E2 Mixing ratio</u> $q_K^2(E0/E2) = \frac{I_K(E0)}{I_W(E2)}$ $q_{K}^{2}(EO/E2)$ can be determined from \Box CE and/or PF intensity, E2: I γ & α_{K} \Box Use ICC and $\Omega(E0)$ values K-shell intensities from other measurements $q_K^2(E0/E2) = \frac{I_{PF}(E0)}{I_{PF}(E2)} \times \frac{\Omega_K(E0)}{\Omega_{PF}(E0)} \times \frac{\alpha_{PF}(E2)}{\alpha_K(E2)}$ X-factor - definition $X(E0/E2) = \frac{B(E0)}{B(E2)} = \rho^2(E0) \times e^2 R^4 / B(E2)$ X-factor - experiment $X(E0/E2) = 2.54 \times 10^9 \times A^{4/3} \times q_K^2 \times \frac{\alpha_K}{\Omega_V} \times E_{\gamma}^5 (MeV)$

Experimental Monopole matrix element $\alpha_{K}(E2)$

$$\rho^{2}(E0) = q_{K}^{2}(E0/E2) \times \frac{\alpha_{K}(E2)}{\Omega_{K}(E0)} \times \lambda_{\gamma}(E2)$$

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E2

Electric monopole (EO) transitions

PHYSICAL REVIEW C

τ

0+

VOLUME 31, NUMBER 4

APRIL 1985

E0 transitions in 82 Kr

1985Ze03

A. Zemel, T. Hageman, J. J. Hamill, and J. van Klinken Kernfysisch Versneller Instituut, 9747 AA Groningen, The Netherlands (Received 9 October 1984)

The first excited 0^+ state of 82 Kr appears to have a noncollective nature, in contrast to the 0_3^+ and other low-spin states in this nucleus. This is corroborated by a conversion-electron measurement of the $0_2^+ \rightarrow 0_1^+$ and the $0_3^+ \rightarrow 0_1^+$ transitions in 82 Kr, following the decay of 82 Rb^g. The values $B(E0;0_2^+ \rightarrow 0_1^+)=3.1(5) \ e^2$ fm⁴ and $X_{311}=B(E0;0_3^+ \rightarrow 0_1^+)/B(E2;0_3^+ \rightarrow 2_1^+)=0.097(24)$ have been deduced from the intensities of the conversion lines, observed with a mini-orange spectrometer. Previous theoretical and experimental investigations of 82 Kr are reviewed.



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```
## python 82Kr_1488E0.py
print "Evaluates E0 transitions from conversion data"
from uncertainties import ufloat
from uncertainties.unumpy import sqrt
from math import pow
##
State='82Kr 1488 E0'
A=82
                                       ## atomic mass
Thalf=ufloat(10E-12,3E-12)
                                      ## half life 10(3) ps
Tau=Thalf/0.6931
                                       ## mean life
print 'State: ', State
## decay data
gK2 E0E2=ufloat(0.087,0.008)
                                   ## E0/E2 mixing ratio
CK_E2=ufloat(0.001031,0.000015)
                                   ## E2 K-conversion coef.
CC_E2=ufloat(0.001163,0.000017)
                                      ## E2 total conversion coef.
## E2 transition
## intensities are in terms of the I K(E2)=1
Eq_E2=0.7112
                                       ## E_gamma [MeV]
IK E2=1.0
                                       ##
IG E2=IK E2/CK E2
                                      ## I_gamma(E2)
IT E2=IG E2*(1+CC E2)
                                       ## I tot(E2)
## E0 transition
IK_E0=IK_E2*qK2_E0E2
                                       ## E0
                                      ## Omega_K(E0)
WK E0=8.473E+8
                                       ## Omega T(E0)
WT E0=9.886E+8
IT E0=IK E0*WT E0/WK E0
                                       ## I_tot(E0)
## X-value
X=2.54E+9*pow(A,1.3333)*qK2_E0E2*(CK_E2/WK_E0)*pow(Eg_E2,5)
print '
        X(E0/E2)=', X
## Partial E2 photon width
Tau_gE2=Tau*(IT_E2+IT_E0)/IG_E2
## Rho**2
r2_E0=qK2_E0E2*CK_E2/(WK_E0*Tau_gE2)
r_E0=sqrt(r2_E0)
                                      ## ENSDF: rho(E0) given
           rho(E0)=', r_E0
print '
```

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T. Kibédi, R.H. Spear / Atomic Data and Nuclear Data Tables 89 (2005) 77-100

2005Ki02

Table 1

Spectroscopic information on $0^+ \rightarrow 0^+$ transitions. See page 95 for Explanation of Table

Nuc	clide	$E_{\rm i}~({\rm keV})$	$T_{1/2}$	Transiti	on		$q_K^2(\mathrm{E0}/\mathrm{E2})$		X(E0/E2)	$10^3 \times \rho^2(\text{E0})$) References	
				J_{i}^{π} – J_{f}^{π}	E0 (keV)	E2 (keV)						
72 36 K	Kr ₃₆	671	26.3 (20) ns	$0^{+}_{2}-0^{+}_{1}$	671	h				71 (6)	[333]	
⁷⁴ ₃₆ Kr ₃₈		509	13.3 (7) ns	$0^{ ilde{+}}_2 - 0^{ ilde{+}}_1$	509	53	1.9 (5)	ABE	0.017 (4)	113 (27)	[282,300,309,333,334]	
⁷⁸ ₃₆ Kr ₄₂		1017.2	2 7.6 (21) ps	$0^+_2 - 0^+_1$	1017	562.1	0.136 (6)	A	0.024 (1)	47 (13)	[262]	
$\frac{80}{36}$ Kr ₄₄		1320.5	6 4.9 (21) ps	$0^+_2 - 0^+_1$	1320.5	703.9	0.103 (11)	A	0.023 (3)	21 (10)	[238]	
⁸² ₃₆ Kr ₄₆		1487.6	10 (<i>3</i>) ps	$0^+_2 - 0^+_1$	1488	711.2	0.087 (8)	E	0.0174 (16)	7.3 (23)	[182,339]	
		2171.7	$\approx 2 \text{ ps}$	$0^+_3 - 0^+_1$	2172	1395.1	0.14 (4)	E	0.10 (3)	≈ 7	[182,339]	
1											- FNSDF	
	82K	R L	1487.62	70+								
	82K	RE		0.04	4 3 0	.0096 7	6.72	4		C	0.054 4	
	82K	RS E	EAV=837.4	33\$CK=0.1	1556 1	5\$CL=0.0	01804 1	8\$CM+	-=0.00370) 4		
	82K	RG	711.2	1 0.38	2 F2							
	82k	R G	1488		 F0					6 2F	-6 6	R
	021 021		$\frac{1}{100}$	6¢ //						0.21	. 0 0	
	021		K/K+L+=0.7									
	82K	KZ G	MR2K(EU/E2)=0.087	8\$							
	82K	R CG		CEK(1488))/CEK(1	(475)=0.	31 3;					
	82K	R2CG	CEK(1488)=	4.7E-6 5	per 10	00 82RB	(1.273	M) (decays (1985Ze03)		
	82K	R CG	MR2K(E0/E2)\$ from	1985ZeC)3						
	82K	R CG		X(E0/E2):	=0.0174	16 (1	985Ze03))				
	82K	R CG		RHO(E0)=	0.086	13 (198	5Ze03)					



Mixed EO+E2+M1 transitions

As for pure EO, but MR(E2/M1) also needed

Conversion coefficient for atomic shell/PF "i" $\alpha_i \ (exp) = \frac{\alpha_i (M1) + (1 + q_i^2) \delta^2 \alpha_i (E2)}{1 + \delta^2}$

 $\frac{X \text{-factor} - experiment}{X(E0/E2)} = 2.54 \times 10^9 \times A^{4/3} \times q_K^2 \times \frac{\alpha_K}{\Omega_K} \times E_{\gamma}^5 (MeV)$ Experimental Monopole matrix element $\rho^2(E0) = q_K^2(E0/E2) \times \frac{\alpha_K(E2)}{\Omega_V(E0)} \times \lambda_{\gamma}(E2)$

$$\frac{EO/E2 \text{ Mixing ratio}}{q_K^2(EO/E2)} = \frac{I_K(E0)}{I_K(E2)}$$

$$\frac{From \alpha_i(exp) \text{ using}}{new \text{ BrIccMixing}}$$



Ω_i(EO) calculations: <u>K, L1, L2, M1, M2, N1, N2...</u> with G. Gosselin, V. Meot, M. Pascal (CEA, France) CATAR (Pauli and Raff (Comp. Phys. Comm. 9 (1975) 392). Modified screening function reduces difference (A.E. Stuchbery, ANU) <u>Pair Formation</u>

Total as well double differential for pair conversion measurements (T.K. Eriksen, ANU)



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1986Su11

198651111

1971Af05

1958Dz01

1959Dz10 1962Ba57 1967Ka12

1962Ba57

1964Pe17

1974Sc03

1973Ca10

1972Gi05

1974Ha63

1974Ha63

2001Kil0

1994Ki01

1994Ki01

1999Da18

1984Co1

1999Le61 1999Le61 1987Va09

1977Dr08

1990Tr01

1970Go09

1985Ra21

1960Lu07

1984Ho02

1984Ho02

1976Mii03

1987Va09,1990Tro

L987Va09,1990Tr0

1987Va09,1990Tr0 1987Va09,1990Tr0 1986Ka07,1990Tr0 1986Ka07,1990Tr0 1986Ka07,1990Tr0

1987Ju06,1990Tr01 1987Ju06,1990Tr01

1987Ju06,1990Tr0:



BrIcc V3.0

- □ Z extended to 126
- \square New $\Omega(\text{EO})$ tables for K, L1, L2, M1, M2 ... shells and PF for Z=6-100
- □ NS_Lib library to parse validate ENSDF records
- □ Monte Carlo propagation of uncertainties
- Technical Meeting on Improvement of Codes used for Nuclear Structure and Decay Data Evaluations, IAEA, 10-13 June 2014 and 5-8 October 2015

Z= 54	Xenon	T	ransition e	00 keV			BrIcc v3.0 (10-Jun-2014)					
Shell	E_e [keV]	Umg(E0) E0	E1	M1	E2	M2	E3	МЗ	E4	M4	E5	M5
Tot		1.729E+10	4.199E-04	1.020E-03	8.226E-04	2.259E-03	1.533E-03	4.196E-03	2.759E-03	7.389E-03	4.875E-03	1.270E-02
K	1365.44	1.499E+10	3.244E-04	8.723E-04	6.975E-04	1.946E-03	1.316E-03	3.600E-03	2.341E-03	6.286E-03	4.038E-03	1.069E-02
L-tot		1.908E+09	3.884E-05	1.068E-04	8.660E-05	2.464E-04	1.737E-04	4.769E-04	3.341E-04	8.804E-04	6.320E-04	1.599E-03
M-tot		2.694E+08	7.807E-06	2.154E-05	1.748E-05	4.990E-05	3.528E-05	9.710E-05	6.842E-05	1.805E-04	1.306E-04	3.303E-04
N-tot		8.489E+07	1.616E-06	4.465E-06	3.615E-06	1.035E-05	7.284E-06	2.012E-05	1.410E-05	3.736E-05	2.684E-05	6.830E-05
0-tot		3.709E+07	2.031E-07	5.632E-07	4.521E-07	1.302E-06	9.023E-07	2.519E-06	1.725E-06	4.645E-06	3.239E-06	8.414E-06
IPF		1.495E-04	4.705E-05	1.455E-05	1.691E-05	5.153E-06					4.484E-05	
TranEne	er ChemSymb	Z+Integer	SUBShell [DATAtable	? for help	EXIT [1400)] >					



The Auger effect Pierre Auger - Lise Meitner



Pierre Victor Auger (1899 - 1993)

P. Auger, C.R.A.S. 177 (1923) 169-171. 1923:

"When the first [atomic] electron leaves [the atom, ejected by an incident X-ray], as a secondary β -ray, there is a vacancy left in the electronic system of the excited atom. The drop of a more peripheral electron on that level is accompanied by the emission of a characteristic radiation quantum. This quantum may be absorbed in the atom itself, and produce, at the expense of the peripheral levels [the outer electronic shells], a tertiary β -ray... The repetition of that process must lead to the production of a fourth order ray; and I in-deed believe I have observed such rays in the case of [gaseous] iodine."



Lise Meitner (1878- 1968)

Auger electrons and X-rays are part of the radiations emitted in nuclear decay! Not in ENSDF

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First multi-electron tracks from photoionization seen in a cloud chamber.



Les points blancs aux origines des rayons β secondaires manifestent l'existence d'un rayonnement mou. (*Tous ces clichés sont grossis environ 2 fois*).

P. Auger Journal de Physique et le Radium, **6** (1925) 205.

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JOURNAL DE PHYSIQUE



The biological effect of Auger electrons

Interaction of ionizing radiation:

- □ Spectrum of energy loss
- □ Generation of secondary electrons
- Low energy electrons are the ideal tool
- Auger electrons from radioisotopes decay at close proximity to the DNA

Which Isotope?

- □ Number of electrons per decay
- **D** Ratio of X & γ vs. e⁻ & β
- Physical vs. effective half life
- Suitable radiochemistry

<u>Physics input</u> to dose calculations:

- Energy loss
- Radiation spectra

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BrIccEmis Initial vacancy creation





ENSDF - Evaluated Nuclear Structure Data File



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23-Mar-2016, 14th IWRDD



Electron capture





Electron capture rates

- $P_{K}+P_{L}+P_{M}+P_{N}+P_{O}=1$
- E. Schonfeld, PTB-6.33-95-2 (1995)

Internal conversion





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□ X-ray or Auger electron emission to fill vacancy

- Multi step, stochastic process; Monte Carlo
- Transition energies and transition probabilities are needed for every propagation step
- □ Transition energies from Dirac-Fock atomic model
 - RAINE code (Band 2002) No QED or Breit corrections

Transition rates from EADL (Perkins 1991)

- Calculated for single initial vacancies
- No shaking or double Auger process
- Krause-Carlson correction to transition rates to take into account multiple vacancies







- □ Multi step, stochastic process; Monte Carlo
- Transition energies and transition probabilities are needed for every propagation step
- □ Transition energies from Dirac-Fock atomic model
 - RAINE code (Band 2002) No QED or Breit corrections
- □ Transition rates from EADL (Perkins 1991)
 - Calculated for single initial vacancies
 - No shaking or double Auger process



STOP: Vacancy in valence shell / no transition is possible





- □ Is the atom ISOLATED or in CONDENSED PHASE?
 - Condensed phase: vacancies filled from environment (Charlton and Booz 1981, Humm 1984, Howell 1992)
- \square Auger cascade very fast: 10⁻¹⁴ to 10⁻¹⁶ s
- □ Neutralization is a slow process (Pomplun 2012)
 - BrIccEmis: fast neutralization and option <u>Correct treatment: condensed physics model</u>



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¹³¹Cs EC - Auger spectrum



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¹³¹Cs EC - Auger spectrum



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nature

materials

LETTERS PUBLISHED ONLINE: 15 JUNE 2015 | DOI: 10.1038/NMAT4323

Enhancement of low-energy electron emission in 2D radioactive films

Alex Pronschinske¹, Philipp Pedevilla², Colin J. Murphy¹, Emily A. Lewis¹, Felicia R. Lucci¹, Garth Brown³, George Pappas³, Angelos Michaelides² and E. Charles H. Sykes^{1*}



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Tufts University, MA, USA



¹²⁵I EC

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Experiment

Pronschinske (2015)

Alex Pronschinske¹, Philipp Pedevilla², Colin J. Murphy¹, Emily A. Lewis¹, Felicia R. Lucci¹, Garth Brown³, George Pappas³, Angelos Michaelides² and E. Charles H. Sykes^{1*}

200

×





2.1e⁻

E. Pomplun et al, Radiat. Res. 111 (1987) 533.





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Charge state distribution of fission isomers



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Charge state distribution of fission isomers



- 55.0 keV isomeric state decays in flight
- Auger cascade increases ionization state by ~5 units of charge

Collaboration: Ulli Köster (ILL) & Grégoire Kessedjian (LPSC)

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99mTc Used for ~30M medical procedures every year

## ELE(TROMAGNETIC	TRANSITIONS =====			2	n		BrlccEmis (L	ee et al. 2012)
# Trans	Energy[keV]	Prob.[per 100 decays	5]		10 ²	^{99m} Tc IT deca	y	Auger	electrons
G-1	140.511(1)	88.80(20)			10 ¹				-
K - 1	119.467	8.86(17)			0		. In all a		1
L-1	137.673	1.080(19)			10 ⁰	F V N/N		.h	
M - 1	140.126	0.196(4)		ays	10 ⁻¹				
N - 1	140.480	0.0311(6)		dec	10				
G - 2	2.1726(15)	7.23E-9(11)		8	10 ⁻²				1
M - 2	1.7879	87.5(11)		er 1	10 ⁻³		NAMATA		
N - 2	2.1422	11.54(16)		/ b€	10				
G –	142.6831(11)	0.0238(4)		r e/	10 ⁻⁴				
K-3	121.6391	0.693(16)		be	10 ²	K-total ——	- 		X-ravs
⊥-Э м и	139.8455	0.810(3)		sity	101	L-total ——— L M-total ———			,
IVI - 0	146.6904	0.04&&(0)		lten	10	N-total ——			
				<u> </u>	10 ⁰	-			
# SIMUL	ATED TOTAL EN	ERGY RELEASED PE	R DECAY======		10 ⁻¹	E I			
# Tran	s En	ergy[keV]			10-2		h	l I	
Gamn	na-Rays:	125.9386			10				
CE ele	ectrons:	15.4571			10 ⁻³	-			
X-rav	'S:	1.4110			10 ⁻⁴				
 	electrong	0.8358			1	0 ⁻³ 10 ⁻²	_10 ⁻¹	10 ⁰	10 ¹
muger	. 010001 0118.	0.0000					Energy [ke	VJ	

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Used for ~30M medical procedures every year



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99mTc



Used for ~30M medical procedures every year

X-ray tran	sition types:	50					BrlccEmis (L	ee et al. 2012)
# # Trang	Energy Mean[keV]	95% Conf range	Prob [ner 100 de	10) ² ^{99m} Tc IT decay		Auger	electrons
X-ray tot	16.8459	[0.0367:20.6725]	1 8.376E+00				•	-
X-ray Ktot	18.7556	[18.3018:21.0567]] 7.457E+00	10		114		-
X-ray KL2	18.3018	[18.3018:18.3018]] 2.153E+00	10	o [\			-
X-ray KL3	18.4207	[18.4207:18.4207] 4.111E+00	s s	-			
X-ray KM	20.6663	[20.6519:20.6725] 9.982E-01	रेषे 10		White here is a second s		
X-ray KM2	20.6519	[20.6519:20.6519]] 3.403E-01	dec				
X-ray KM3	20.6725	[20.6725:20.6725	5] 6.532E-01	g 10	-2 - ^^.			
X-ray KN	21.0614	[21.0567:21.0638]] 1.940E-01	10		li li li di <mark>Ma</mark> ta		
X-ray KN2	21.0567	[21.0567:21.0567] 6.800E-02	<u>a</u> 10	-3 E 10 I II	(MANANALA,		
X-ray KN3	21.0638	[21.0638:21.0638] 1.257E-01	>	-1	1 V IT 'N I' II I V		
X-ray Ltot	2.4651] 4.869E-01	ື _ພ 10		// · // · // · //	└╷╷┛╷╝	
X-ray Mtot] I.016E-01	ă 10) ² K-total ——	·	·	X-rays
x-ray intot	0.0351	0.0278: 0.0403	」 3.304世-01	sity	L-total ——			-
				L 10	N-total —			
				드 10) ⁰ -			
				10	-1			
				10	-2	ь		
New	ENSDF C	ard(s) to hold a	itomic	10	Ē	11 հե		
radi	ations.			10	-3 [
Tmm	ediately t	before the P/N/	G/L card			<mark></mark>		
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Tibor Kibèdi, Dep. of Nuclear Physics, Australian National University

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ICTP-IAEA ENSDF workshop, Trieste, August 2016

Energy [keV]

99mTc



Summary and outlook

<u>Future plans</u>

- Atomic transitions energies and rates from Grasp2K/RATIP and MCDFGME (ANU-Malmo-Lisbon collaboration)
- Low energy (100 eV to 4 keV) Auger electron measurements to benchmark calculations
- Condensed phase physics input to incorporate environmental effects



Collaborators

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