Inorganic Chemistry
including bioinorganic chemistry

Supporting Information for *Inorg. Chem.*, **1994**, 33(6), 1165-1170, DOI: 10.1021/ic00084a032

CHAKRABARTI
1165-1170

Supplementary Material P-1170-M1

BEKZOG	Heistand et al	Inorg. Chem. 21, 676 (1982)
BILRIX	Zozulin et al	Inorg. Chem. 21, 3083 (1982)
BIWMOJ	Quingchuan et al	Sci. Sin. (Eng.Ed.) B25, 356 (1982)
BONDIR	Pasquali et al	J. Chem.-Soc. Chem. Comn., 197 (1983)
BORSOQ	Edwards et al	J. Am. Chem. Soc. 103, 7792 (1981)
BOYLUW	Wenrui et al	J. Struct. Chem. 1, 73-1 (1982)
CAPGAB	Cleland et al	J. Am. Chem. Soc. 105, 6021 (1983)
CAZFAK	Coffindaffer et al	Inorg. Chem. 22, 3178 (1983)
CINHIQ	Boersma et al	J. Organomet. Chem. 81, 7 (1974)
CIYLAX	Kanatzidis et al	J. Am. Chem. Soc. 106, 4500 (1984)
CIYLEB	as above	
CLPHTI	Watenpaugh et al	Inorg. Chem. 5, 178 (1966)
COLNIA	Collman et al	J. Am. Chem. Soc. 106, 5151 (1984)
CUDWUT	Zaworotko et al	Organometallics 4, 238 (1985)
CUDXAA	as above	
CUTDOK	Jolibois et al	Inorg. Chim. Acta 97, 119 (1985)
CUTKIL	Lewis et al	Inorg. Chem. 24, 363 (1985)
DAJHEB	Beringhelli et al	J. Chem. Soc. Dalton, 1507 (1985)
DASCAB	Coffindaffer et al	J. Am. Chem. Soc. 107, 3572 (1985)
DAXSEA	Coffindaffer et al	J. Chem. Soc. Chem. Com., 1519 (1985)
DAXSIE	as above	
DAXSOK	as above	
DIBJUT	Rees et al	Organometallics 4, 2179 (1985)
DILTAT	Hayashi et al	J. Am. Chem. Soc. 108, 385 (1986)
DOPYOW	Fiaschi et al	Inorg. Chem. 25, 462 (1986)
DUBTEZ	Fryzuk et al	Can. J. Chem. 64, 174 (1986)
DUNSOU	Fraser et al	Can. J. Chem. 64, 816 (1986)
DUNSUA	as above	
ETYNWB	Chiu et al	J. Chem. Soc. Dalton, 1204 (1981)
FAKJEG	Mazzanti et al	Inorg. Chem. 25, 4158 (1986)
FEXBEP	Nasri et al	J. Am. Chem. Soc. 109, 2549 (1987)
FOTBAR	Braga et al	J. Organomet. Chem. 334, C46 (1987)
FUJHIB	Kegley et al	J. Am. Chem. Soc. 109, 6563 (1987)
GANZIE	Fraser et al	Can. J. Chem. 65, 2558 (1987)
GANZOK	as above	
GIBCUP	Salifoglou et al	Inorg. Chem. 27, 3394 (1988)
GIMREZ	Darensbourg et al	Inorg. Chem. 27, 3269 (1988)
GINGIT	Erikson et al	Organometallics 7, 1930 (1988)
JAFGUS	Murchie et al	Can. J. Chem. 66, 2515 (1988)
JECHUU	Kim et al	J. Am. Chem. Soc. 112, 1096 (1990)
JECJAC	as above	
JECJEG	as above	
JECJIK	as above	
KARKUJ	Erker et al	Organometallics 8, 2037 (1989)
KARVUU	Cowan et al	J. Am. Chem. Soc. 111, 4750 (1989)
KECBUP	Bernard et al	Organometallics 9, 12 (1990)
KEXDIA	Watson et al	Can. J. Chem. 68, 1201 (1990)
MEORHC	Edwards et al	J. Chem. Soc. Dalton, 2467 (1980)
PHOECU	Calderazzo et al	J. Chem. Soc. Dalton, 1419 (1980)

SABKOV	Wilisch et al	Inorg. Chem. 27, 4333 (1988)
SEBTUO	Darensbourg et al	J. Am. Chem. Soc. 111, 7094 (1989)
SENPAC	Osakada et al	J. Organomet. Chem. 382, 303 (1990)
SERMIL	Bhaduri et al	J. Chem. Soc. Dalton, 1305 (1990)
SIDPIE	Drake et al	Inorg. Chem. 29, 2707 (1990)
TPOXTI10	Svetich et al	Acta Cryst. B28, 1760 (1972)
VANNED	Kipke et al	Acta Cryst. C45, 870 (1989)
VEGYIP	Al-Ahmad et al	Inorg. Chem. 29, 927 (1990)
VEGZAI	as above	

P-1170-MS

RELEVANT PORTIONS OF GSTAT89 OUTPUT CONTAINING REFCODE, ANGLES MOC, THETA AND PHI, AND THE CATION PRESENT. THE CONVENTION OF PHI (PRINTED HERE AND USED IN THE PAPER) IS DIFFERENT FROM THAT IN CSD: PHI(PAPER) = 90 - PHI(CSD)

BEKZOG	132	58	38	FE
BILRIX	125	39	24	U
	119	30	12	
	163	86	16	
	126	36	6	
	174	88	6	
	158	79	19	
	132	46	21	
BIWMOJ	177	88	2	ZR
	153	84	26	
BONDIR	129	84	51	CU
	128	74	50	
BORSOQ	167	79	6	U
	162	72	2	
	165	82	13	
	166	86	13	
BOYLUW	153	86	27	ZR
CAPGAB	133	79	46	FE
	129	87	51	
	132	84	47	
	123	55	49	
CAZFAK	138	74	39	MO
	138	77	40	
	139	80	40	
	144	81	35	
	135	74	43	
	135	68	40	
	141	84	39	
	145	84	35	
	141	77	37	
	135	81	43	
CINHIQ	126	69	51	ZN
	117	27	1	
	118	63	58	
CIYLAX	107	72	72	FE
CIYLEB	126	81	54	FE
CLPHTI	123	33	6	TI
	166	88	14	
	128	39	5	
COLNIA	128	38	1	RU
	132	42	5	
CUDWUT	116	30	29	AL
	117	30	25	
CUDXAA	125	51	42	
	125	53	44	
CUTDOK	122	34	17	SN
	126	37	13	
	123	36	22	
	123	34	9	
CUTKIL	126	38	13	TA
	156	78	21	
	144	67	29	
	166	83	13	
	148	70	26	

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	122	32	8	
DAJI EB	130	77	49	RE
	135	83	44	
	131	90	49	
	132	84	48	
	129	83	50	
	134	88	46	
DASCAB	140	73	37	MO
	132	46	22	
	141	53	13	
	143	64	27	
	135	63	38	
	139	65	34	
	146	65	24	
	143	71	32	
DAXSEA	171	83	16	NB
	156	69	10	
DAXSIE	177	90	3	NB
	169	82	8	
	150	75	26	
	143	89	37	
	146	73	30	
	161	85	18	
	153	71	20	
	148	67	22	
DAXSOK	160	78	16	NB
DIBJUT	127	86	53	IR
DILTAT	138	48	5	CO
DOPYOW	128	89	52	CU
DUBTEZ	120	48	48	RH
	117	51	54	
DUNSOU	121	56	51	K
	108	29	49	
DUNSUA	129	87	51	NA
	120	40	38	
	146	74	30	
	131	75	47	
ETYNWB	142	90	38	W
FAKJEG	133	43	5	V
FEXBEP	138	82	42	FE
FOTBAR	121	67	57	PD
FUJHIB	122	86	58	RH
GANZIE	122	87	58	K
GANZOK	125	68	51	NA
GIBCUP	135	67	40	FE
	143	88	37	
	130	44	22	
	134	65	40	
GIMREZ	134	85	46	W
	131	81	48	
	132	85	47	
	129	78	50	
	131	74	46	
	131	89	49	
GINGIT	125	62	50	RE
JAFGUS	131	61	41	LI
	120	89	60	
	141	56	20	LI
	138	84	42	

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JECHUU	121	83	58	PD
JECJAC	122	86	58	NI
JECJEG	127	89	53	PD
JECJIK	125	88	56	PD
KARKUJ	155	73	19	ZR
KARVUU	124	90	56	PT
KECBUP	126	83	54	RH
KEXDIA	139	84	40	LI
	139	82	41	
	140	79	39	
	135	65	38	
MEORHC	141	73	35	RE
	132	53	33	
PHOECU	129	43	24	CU
	120	55	53	
	134	85	46	
SABKOV	141	64	30	V
	134	44	3	
	120	71	58	LI
	124	43	34	
SEBTUO	132	75	47	W
	130	82	49	
SENPAC	120	88	60	PT
SERMIL	128	69	49	RU
	129	68	48	
	129	70	48	
	128	71	49	
	116	26	3	
	116	26	4	
SIDPIE	108	41	62	SR
	131	53	34	
	133	52	30	
	138	54	23	
	133	86	47	
	120	33	22	
	135	63	37	
	106	37	63	
	115	26	9	
TPOXTI10	132	59	38	TI
	169	86	10	
	126	42	29	
	127	46	34	
	175	85	2	
	125	44	34	
VANNED	135	74	43	MO
	137	55	27	
VEGYIP	143	89	37	FE
	137	77	41	
	129	40	12	
	130	87	50	
	130	86	50	
	130	68	47	
VEGZAI	134	68	42	FE
	146	78	32	
	134	75	44	

OUTPUT FROM GSTAT89, CONTAINING VARIOUS CATION COORDINATES EXPRESSED IN TERMS OF THE MOLECULAR COORDINATE SYSTEM (THE FIRST FEW RECORDS ARE FOR THE PHENOLATE GROUP).

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V-1170-M9

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ATOM    FE3     1.32389 1.29997 0.50427
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COMMent connectivity search; screened for any metal (28), error
COMMent free at .02A (32), no disorder (35), coordinates present
COMMent (153), oxygen present (256)
SAVE 2 3
STOP 600
SCREEN 28 32 35 153 256
T1 *CONNser
Q Metal-phenolate
AT1  4M 1
AT2 O 2 0
AT3 C 3 0 E
AT4 C 2 1 E
AT5 C 2
AT6 C 2
AT7 C 2
AT8 C 2 1 E
BO 1 2 99
BO 2 3 1
BO 3 4 5
BO 4 5 5
BO 5 6 5
BO 6 7 5
BO 7 8 5
BO 3 8 5
NOLN
END
QUEStion T1
```

GEOMETRY CALCULATION USING GSTAT89 (PLEASE NOTE THAT THETA AND TETA ARE EQUIVALENT AND THE CALCULATION OF TETA IS REDUNDANT):

```
BRI
COD
NOD
FRAG Metal-phenolate
AT1 4M 1 #
AT2 O 2
AT3 C 3 E
AT4 C 2
AT5 C 2
AT6 C 2
AT7 C 2
AT8 C 2
BO 1 2
BO 2 3
BO 3 4
BO 4 5
BO 5 6
BO 6 7
BO 7 8
BO 3 8
TEST DIST 1 2 1.5 3.2
NOL
END
DEF M-O 1 2
DEF MOC 1 2 3
SETUP P1 2 3 4 5 6 7 8
DEF DIST 1 P1
SETUP V1 2 1
DEF TETA V1 P1
DEF *LP2 THETA PHI 4 3 2 1
DEF *RFACT
DEF *AS
DEF *ERR
HIST MOC
SCAT THETA PHI
OUTPUT COORD ORIG 2 XM 3 2 YM 4 8
SUP AVE
```