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Structure of Bis[1,2-bis(diphenylphosphinoethylene)]iodocobalt(II) Tetraphenylborate

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Abstract. $[\mathrm{CoI}(\mathrm{C_{26}H_{22}P_2})_2][\mathrm{B}(\mathrm{C_6H_5})_4]$, $M_r = 1297{\cdot}9$, monoclinic, $P2_1/c$, $a = 21{\cdot}014\,(3)$, $b = 13{\cdot}223\,(3)$, $c = 24{\cdot}696\,(5)$ Å, $\beta = 110{\cdot}9\,(2)°$, $V = 6411\,(5)$ Å^3, $Z = 4$, D_m(by flotation) = 1·35, $D_x = 1{\cdot}345$ g cm^{-3}, $\lambda(\mathrm{Mo}\,K\alpha) = 0{\cdot}71069$ Å, $\mu = 8{\cdot}818$ cm^{-1}, $F(000) = 2660$, $T = 293$ K. Final $R = 0{\cdot}074$ for 3886 unique reflections. The geometry around cobalt is a distorted trigonal bipyramid in which each diphos ligand bridges an axial and an equatorial position and the iodine atom occupies an equatorial position. There is tetrahedral geometry around the B atom.

Introduction. The vacant 3*d* orbitals of the P atom are capable of interacting with filled non-bonding *d* orbitals of transition metals. Phosphines act as σ-bond donors and π-bond acceptors. The stabilizing effect of phosphine ligands has been utilized in the preparation of a wide range of stable organometallic compounds.

On the basis of ESR and electronic spectra, the geometry around cobalt in the cation of $[\mathrm{Co}\{(\mathrm{C_6H_5})_2\mathrm{PCH_2CH_2P}(\mathrm{C_6H_5})_2\}_2\mathrm{Cl}]\mathrm{SnCl_3.C_6H_5Cl}$ (Horrocks, Hecke & Hall, 1967) was suggested as square pyramidal, but X-ray analysis showed a trigonal bipyramidal geometry with two of the P atoms occupying the axial positons and two P atoms and one Cl atom forming the equatorial plane (Stalick, Corfield & Meek, 1973).

Experimental. The compound was prepared by the procedure followed by McAuliffe & Meek (1969) for the analogous nickel(II) complex. Unit-cell parameters obtained by least-squares refinement of θ values of 25 high-angle reflections. Crystals 0·35 × 0·45 × 0·625 mm, three-dimensional intensity data collected on an Enraf–Nonius CAD-4 diffractometer with graphite-monochromated Mo*Kα* radiation, $\omega/2\theta$ scan mode, standard reflections (222, 133) showed no significant change. All reflections (h: $-19\rightarrow18$, k: $0\rightarrow13$, l: $0\rightarrow20$) in the range $1 < \theta < 25°$ measured; maximum counting time for a reflection 60 s, 5683 reflections measured, 3886 unique reflections with $I > 3\sigma(I)$ considered observed; intensities not corrected for absorption. Structure was solved by heavy-atom method and refined by full-matrix least squares, minimizing $\sum w|\Delta F|^2$ with *SHELX*76 (Sheldrick, 1976), initially with isotropic and then anisotropic thermal parameters for non-H atoms of the cation. Refinements of 587 positional and thermal parameters including the scale factor converged to $R = 0{\cdot}074$. Maximum and average shift/e.s.d. are 0·38 and 0·27 respectively except for C(28), whose thermal parameter became non-positive-definite and the shift/e.s.d. was 0·87. Final difference Fourier maps revealed the positions of 15 of the 64 H atoms. These were refined for one cycle. Maximum peak in final difference Fourier map is 0·98 e Å^{-3}, $wR = 0{\cdot}074$, $w = 1{\cdot}00/[\sigma^2(F_o) + 0{\cdot}0007|F_o|^2]$.

Atomic scattering factors for non-H atoms from Cromer & Mann (1968), anomalous-dispersion correction factors from Cromer & Liberman (1970), H-atom scattering factors from Stewart, Davidson & Simpson (1965).

Discussion. Atomic coordinates with equivalent isotropic thermal parameters are listed in Table 1.* Table

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* Lists of structure factors, H-atom coordinates, anisotropic thermal parameters, bond distances and angles, and atom-to-plane distances have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44801 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Final fractional coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* (Å^2 $\times$ 10^4 *for* Co, I *and* Å^2 $\times$ 10^3 *for others*) *with e.s.d.'s in parentheses*

$U_{\rm eq} = \frac{1}{3}\sum_{i=1}^{3} U_{ii}$. Atoms following B have been refined isotropically.

	x	y	z	$U_{\rm eq}/U_{\rm iso}$
I	494 (1)	2267 (1)	4416 (1)	419 (8)
Co	1776 (1)	2590 (2)	4922 (2)	283 (13)
P(1)	1699 (2)	2599 (3)	5809 (2)	32 (3)
P(2)	2684 (3)	1567 (3)	5382 (2)	37 (3)
P(3)	1940 (3)	2539 (3)	4066 (2)	33 (3)
P(4)	2284 (3)	4150 (3)	5009 (2)	33 (3)
C(1)	2582 (9)	2532 (11)	6320 (7)	37 (11)
C(2)	1315 (9)	1561 (11)	6053 (7)	32 (11)
C(3)	1305 (9)	3700 (12)	6036 (7)	35 (11)
C(4)	3034 (10)	2040 (11)	6124 (8)	49 (12)
C(5)	2463 (10)	270 (13)	5514 (8)	44 (12)
C(6)	3427 (9)	1408 (13)	5173 (7)	40 (11)
C(7)	2129 (9)	1330 (12)	3808 (7)	39 (11)
C(8)	2674 (9)	3363 (13)	4140 (7)	40 (11)
C(9)	1292 (10)	3010 (12)	3410 (8)	38 (12)
C(10)	2812 (9)	4062 (13)	4560 (8)	41 (11)
C(11)	2843 (8)	4665 (12)	5711 (7)	31 (10)
C(12)	1782 (9)	5285 (12)	4666 (7)	36 (10)
C(13)	598 (12)	1488 (22)	5826 (9)	44 (19)
C(14)	265 (11)	674 (17)	6001 (10)	70 (15)
C(15)	660 (10)	−81 (16)	6385 (15)	59 (14)
C(16)	1362 (11)	−5 (13)	6603 (8)	63 (13)
C(17)	1697 (10)	827 (13)	6448 (8)	41 (12)
C(18)	926 (9)	4384 (13)	5625 (8)	42 (13)
C(19)	669 (9)	5244 (13)	5780 (8)	50 (13)
C(20)	760 (10)	5368 (15)	6379 (10)	60 (14)
C(21)	1174 (12)	4706 (18)	6798 (10)	76 (17)
C(22)	1413 (11)	3823 (15)	6637 (9)	61 (15)
C(23)	1776 (11)	−60 (13)	5277 (8)	49 (13)
C(24)	1618 (14)	−1045 (14)	5399 (9)	97 (17)
C(25)	2122 (14)	−1699 (19)	5742 (11)	92 (18)
C(26)	2793 (16)	−1365 (17)	6009 (11)	113 (20)
C(27)	3023 (13)	−334 (16)	5878 (9)	81 (17)
C(28)	3449 (9)	566 (13)	4832 (7)	44 (12)
C(29)	4004 (12)	435 (21)	4626 (10)	76 (19)
C(30)	4508 (13)	1188 (24)	4786 (11)	81 (20)
C(31)	4499 (13)	1991 (21)	5113 (13)	109 (21)
C(32)	3916 (10)	2119 (15)	5342 (10)	82 (16)
C(33)	2568 (11)	1235 (15)	3504 (9)	62 (15)
C(34)	2675 (12)	306 (17)	3260 (9)	75 (16)
C(35)	1811 (12)	−467 (15)	3629 (9)	76 (16)
C(36)	2271 (11)	−521 (14)	3330 (9)	51 (15)
C(37)	1751 (10)	490 (13)	3868 (8)	49 (12)
C(38)	806 (10)	2358 (14)	3046 (8)	49 (13)
C(39)	285 (11)	2717 (17)	2530 (9)	77 (15)
C(40)	244 (13)	3739 (19)	2398 (9)	72 (17)
C(41)	736 (14)	4425 (17)	2776 (12)	76 (19)
C(42)	1260 (11)	4067 (14)	3278 (8)	53 (14)
C(43)	3553 (10)	4464 (13)	5900 (8)	50 (13)
C(44)	3987 (17)	4775 (19)	6462 (5)	57 (32)
C(45)	3716 (17)	5233 (22)	6817 (12)	97 (23)
C(46)	2995 (14)	5475 (18)	6635 (9)	72 (17)
C(47)	2575 (10)	5177 (13)	6053 (8)	51 (13)
C(48)	2137 (10)	6217 (12)	4742 (7)	41 (11)
C(49)	1769 (12)	7082 (14)	4487 (9)	50 (15)
C(50)	1075 (11)	7047 (14)	4184 (8)	49 (13)
C(51)	731 (11)	6132 (16)	4120 (9)	45 (14)
C(52)	1098 (9)	5231 (13)	4367 (8)	44 (12)
B	6476 (14)	1342 (19)	1617 (11)	54 (7)
C(53)	6431 (10)	86 (14)	1749 (8)	52 (5)
C(54)	7208 (9)	1732 (13)	1968 (8)	34 (5)
C(55)	5860 (12)	1918 (17)	1818 (8)	74 (7)
C(56)	6273 (10)	1528 (14)	915 (8)	53 (5)
C(57)	7411 (9)	2238 (14)	2541 (7)	44 (5)
C(58)	7022 (9)	−1523 (13)	2212 (7)	73 (5)
C(59)	6340 (9)	−2002 (13)	1990 (8)	64 (7)
C(60)	5791 (8)	−1491 (11)	1686 (7)	72 (6)
C(61)	5772 (8)	−415 (13)	1578 (9)	117 (6)
C(62)	8050 (9)	2541 (11)	2843 (9)	50 (7)
C(63)	8579 (8)	2400 (12)	2630 (8)	49 (7)
C(64)	8449 (10)	1939 (11)	2116 (9)	43 (8)
C(65)	7770 (9)	1606 (12)	1799 (7)	54 (5)
C(66)	5703 (9)	1608 (11)	2287 (9)	132 (9)
C(67)	5213 (17)	2155 (25)	2476 (14)	121 (9)
C(68)	4974 (15)	2942 (23)	2207 (13)	108 (9)
C(69)	5131 (18)	3393 (28)	1785 (15)	124 (12)
C(70)	5627 (16)	2811 (24)	1579 (13)	121 (10)

Table 1 (*cont.*)

	x	y	z	$U_{\rm iso}$
C(71)	6482 (10)	2425 (15)	715 (8)	47 (6)
C(72)	6351 (12)	2615 (16)	161 (9)	74 (7)
C(73)	5945 (11)	1944 (17)	−292 (9)	64 (6)
C(74)	5731 (11)	1073 (16)	−115 (9)	61 (6)
C(75)	5907 (9)	827 (14)	504 (18)	52 (5)
C(76)	7023 (10)	−451 (15)	2079 (8)	57 (6)

Table 2. *Bond lengths* (Å) *and bond angles* (°) *involving* Co, I, P *and* C *atoms immediately attached to* P *atoms, and* B *and its immediate coordination*

I—Co	2·569 (5)	Co—P(1)	2·253 (7)
Co—P(2)	2·283 (6)	Co—P(3)	2·261 (8)
Co—P(4)	2·297 (5)	P(1)—C(1)	1·837 (17)
P(1)—C(2)	1·801 (18)	P(1)—C(3)	1·857 (19)
P(2)—C(4)	1·824 (19)	P(2)—C(5)	1·836 (19)
P(2)—C(6)	1·823 (22)	P(3)—C(7)	1·817 (18)
P(3)—C(8)	1·843 (19)	P(3)—C(9)	1·815 (17)
P(4)—C(10)	1·831 (24)	P(4)—C(11)	1·843 (16)
P(4)—C(12)	1·856 (16)	B—C(53)	1·70 (3)
B—C(54)	1·56 (3)	B—C(55)	1·72 (4)
B—C(56)	1·65 (3)		

I—Co—P(1)	92·7 (3)	I—Co—P(2)	133·5 (3)
I—Co—P(3)	91·3 (3)	I—Co—P(4)	123·3 (3)
P(1)—Co—P(2)	81·7 (3)	P(1)—Co—P(3)	175·4 (3)
P(1)—Co—P(4)	95·0 (3)	P(2)—Co—P(3)	93·9 (3)
P(2)—Co—P(4)	103·2 (3)	P(3)—Co—P(4)	84·5 (3)
Co—P(1)—C(1)	105·2 (6)	Co—P(1)—C(2)	121·1 (7)
Co—P(1)—C(3)	119·5 (7)	Co—P(2)—C(4)	105·2 (8)
Co—P(2)—C(5)	115·0 (8)	Co—P(2)—C(6)	125·1 (7)
Co—P(3)—C(7)	118·7 (7)	Co—P(3)—C(8)	106·9 (7)
Co—P(3)—C(9)	120·6 (8)	Co—P(4)—C(10)	103·7 (7)
Co—P(4)—C(11)	122·8 (7)	Co—P(4)—C(12)	123·6 (7)
C(1)—P(1)—C(2)	101·3 (8)	C(1)—P(1)—C(3)	106·3 (8)
C(2)—P(1)—C(3)	101·2 (8)	C(4)—P(2)—C(5)	100·3 (9)
C(4)—P(2)—C(6)	104·2 (9)	C(5)—P(2)—C(6)	103·8 (9)
C(7)—P(3)—C(8)	106·0 (8)	C(7)—P(3)—C(9)	100·2 (9)
C(8)—P(3)—C(9)	102·7 (9)	C(10)—P(4)—C(11)	103·0 (9)
C(10)—P(4)—C(12)	97·5 (9)	C(11)—P(4)—C(12)	101·5 (8)
C(53)—B—C(54)	109·1 (17)	C(54)—B—C(55)	106·1 (18)
C(55)—B—C(56)	107·3 (18)	C(53)—B—C(56)	109·6 (17)
C(53)—B—C(55)	112·8 (18)	C(54)—B—C(56)	111·6 (17)

2 contains the interatomic distances and angles. Figs. 1 and 2 show respectively the *ORTEP* plots (Johnson, 1965) of the anion and cation with atom-numbering schemes.

Cation. The coordination geometry around the Co atom can be described as distorted trigonal bipyramidal. Each of the phosphine ligands bridges an axial P and an equatorial P atom. P(1) and P(3) occupy the axial positions and P(2), P(4) and I form the equatorial plane of the trigonal bipyramid. The root mean square deviation of the atoms from the equatorial plane is 0·004 (4) Å and the deviation of the Co atom from the equatorial plane is 0·007 (4) Å. The Co, I and the two axial P atoms form a plane, the mean deviation of the atoms from this plane being 0·016 (3) Å. The angle between these two planes is 97·2 (3)°. P(1)—Co—P(3) is nearly linear [175·4 (3)°]. Average P_a—Co—P_e 88·7 (2) and P_a—Co—I 91·6 (1)° [P_a: axial phosphorus atoms P(1) or P(3) and P_e: equatorial phosphorus atoms P(2) or P(4)] indicate P(1)—Co—P(3) is nearly normal to the equatorial plane. The symmetry at the equatorial plane cannot be approximated to D_{3h}, because of large angular deviations from the threefold symmetry. The significant differences in the bite and non-bite angles [bite 81·7 (3) and 84·5 (3)°, and non-bite 93·9 (3) and 95·1 (3)°] also contribute to the distortion in the trigonal bipyramidal geometry around Co. The distortions can be attributed to unequal atoms in the equatorial plane. Similar distortions were observed in chlorotris[(*o*-diphenylphosphinophenyl)-phosphine]cobalt(II) tetraphenylborate (Blundell & Powell, 1971), dibromotris(1,2-bisdiphenylphosphinoethane)cobalt(II) trichlorostannate(II) chlorobenzene (Horrocks, Hecke & Hall, 1967) and bromobis[1,2-bis(diphenylphosphino)ethylene]cobalt(II) tetraphenylborate (Mahadevan, Seshasayee, Sethulakshmi & Manoharan, 1985).

The axial Co—P distances [2·253 (7) and 2·261 (8) Å] are equal within experimental error and are significantly shorter than the equatorial Co—P bond lengths [2·284 (6) and 2·297 (5) Å]. Similar variations were observed in [Co(qp)Cl][BPh_4] (Blundell & Powell, 1971) who discussed this in terms of crystal-field stabilization energy. Accordingly in C_3 symmetry the d_z orbital is considerably destabilized compared with the other orbitals and thus for a d^7 electron configuration in a Co^{II} complex this orbital will be unoccupied. This leads to a decrease in the axial bond length and an increase in the equatorial bond length which will increase the energy of the d_z^2 orbital, but stabilize the occupied orbitals.

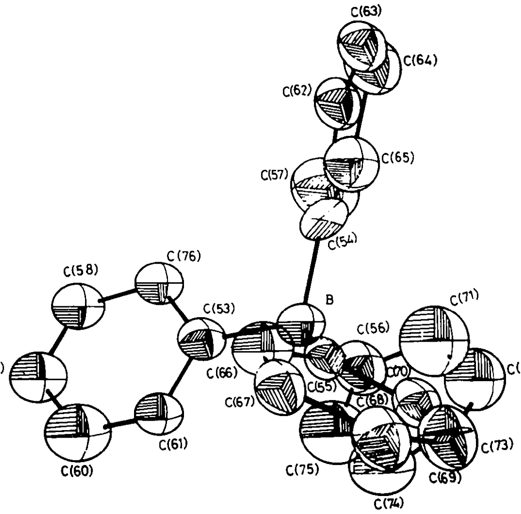

Fig. 1. Perspective view of the anion.

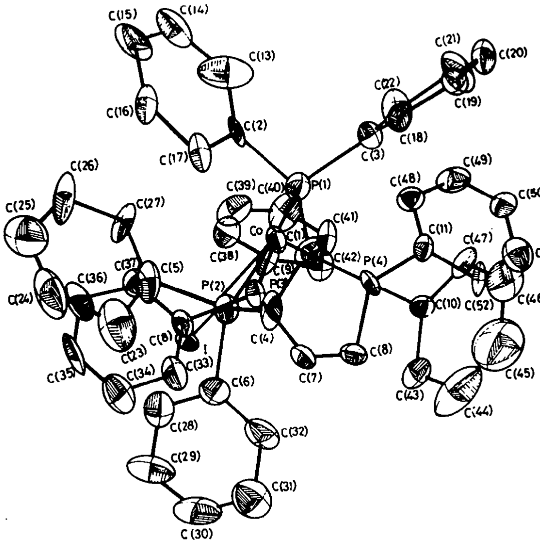

Fig. 2. Perspective vew of the cation.

Table 3. *Comparison of bond lengths* (Å) *and bond angles* (°) *within the coordination sphere of* Co *in* Co(*diphos*$_2$*X*)*Y*

	CoP_4Cl	CoP_4Br	CoP_4I
Co—*X*	2·251 (5)	2·369 (4)	2·569 (5)
$(Co—P)_{av}$	2·258 (5)	2·281 (7)	2·273 (7)
P_a—Co—P_a	176·2 (2)	174·3 (4)	175·4 (3)
P_a—Co—P_e	91·4 (2)	91·8 (3)	88·7 (3)
P_e—Co—P_e	105·7 (2)	96·4 (3)	102·0 (3)
P_a—Co—I	92·3 (2)	87·5 (3)	92·0 (3)
P_e—Co—I	127·1 (3)	131·8 (2)	129·0 (3)

P_a: axial phosphorus atom [P(1) or P(3)].
P_e: equatorial phosphorus atom [P(2) or P(4)].

The Co—I bond length is close to the sum of the covalent radii of cobalt and iodine of 2·58 Å. A comparison of bond parameters within the coordination sphere of cobalt in various Co(diphos$_2$*X*)*Y* species is presented in Table 3.

P—C distances vary from 1·80 (1) to 1·85 (1) Å, which are in the range reported for single-bond lengths. There is an approximate tetrahedral configuration around the P atom with an average C—P—C angle of 102·6 (9)°. The sp^3 hybridization is exhibited by the P atom as shown by the bond parameters around it.

The dihedral angles between the two phenyl groups attached to the axial phosphines [86·97° for P(1) and 88·46° for P(3)] are close to 90°, suggesting that these phenyl groups attached to the axial phosphines enter the *d–p π* bonding with different *p* orbitals. For the two phenyl groups attached to the equatorial phosphines, the dihedral angles are 68·12 and 71·91°, showing that the steric crowding would be larger in the vicinity of these phosphines.

The two five-membered rings are not planar. This may be due to distortion in the tetrahedral configuration around the P atom.

The short intramolecular contacts (<4·00 Å, the van der Waals distance) between I and some C atoms of the phenyl rings are I···C(2) 3·877, I···C(9) 3·576, I···C(13) 3·586 and I···C(38) 3·668 Å, indicating the possibility of steric repulsion, which could be the possible reason for the large deviation from 120° of I—Co—P_e angles.

Anion. The B atom exhibits tetrahedral geometry with C_{ph}—B—C_{ph} angles varying from 106·1 (17) to 112·8 (18)°, the average being 109·4 (16)°, corresponding to an ideal tetrahedral angle. The average $\mathrm{B—C_{ph}}$ bond distance is 1·66 (3) Å. These bond parameters compare well with those obtained in other tetraphenylborates reported (Blundell & Powell, 1971; Cromer & Huneke, 1978; Duggan & Hendrickson, 1974; Bacci & Chilardi, 1974; Sime, Dodge, Zalkin & Templeton, 1971; Glidewell & Holden, 1982).

The B atom deviates significantly from the plane of the phenyl rings, the maximum deviation being 0·83 (2) Å. The four phenyl groups are planar to within 0·029 (2), 0·006 (2), 0·027 (3) and 0·016 (2) Å.

Intermolecular features. There are some short contacts between the cation and the anion of length less than 3·7 Å, namely C(10)···C(76) 3·60 (3), C(64)···C(36) 3·65 (4), C(65)···C(36) 3·69 (4) Å.

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The Structure of 7,14-Di-*n*-propylacenaphtho[1,2-*k*]fluoranthene

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Abstract. $C_{32}H_{26}$, $M_r = 410·26$, monoclinic, $C2/c$, $a = 18·727\,(3)$, $b = 5·149\,(2)$, $c = 24·078\,(4)$ Å, $\beta = 109·67\,(1)°$, $V = 2186·4\,(4)$ Å^3, $D_m = 1·26\,(1)$ (by flotation in $ZnSO_4$ solution), $D_x = 1·247$ Mg m^{-3}, $\mu(\mathrm{Cu}\,K\alpha) = 0·50$ mm^{-1}, $Z = 4$, $\lambda(\mathrm{Cu}\,K\alpha) = 1·5418$ Å, $F(000) = 872$. Final $R = 0·048$ for 1717 observed diffractometer data. The molecule is nonplanar and is closely related to 7,14-di-*n*-butylacenaphtho[1,2-*k*]fluoranthene and 7,14-di-*n*-pentylacenaphtho[1,2-*k*]fluoranthene. The propyl group is almost planar [to within ±0·035 (3) Å] forming a zigzag arrangement pointing along **c** and perpendicular to the needle axis **b**. It has normal configuration and dimensions, with C—C distances varying from 1·505 (3) to 1·531 (4) Å. The atoms of the fluoranthene moiety are coplanar to within ±0·050 (2) Å; the plane of the propyl group is almost perpendicular to it. Molecules are held together by van der Waals interactions. Bond lengths and angles are in reasonable agreement with those obtained in other 7,14-disubstituted acenaphtho[1,2-*k*]fluoranthenes.

Introduction. The crystal structure of the medium-sized nonalternant hydrocarbon fluoranthene has already been determined by X-ray and neutron diffraction (Hazell, Jones & Sowden, 1977). The structures of the 7,14-disubstituted acenaphtho[1,2-*k*]fluoranthenes (I), (II) and (III), determined from X-ray photographic and counter diffractometer data (Seth & Chakraborty,

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