Table 33A-9-001. CsD_2AsO_4 (DCDA). Fractional coordinates and anisotropic temperature parameters [81Hay]. The values on the first line for each atom are for T = RT, and those on the second line are for $T = \Theta_f + 5$ K (Θ_f = 210 K). The anisotropic temperature parameters U_{ij} (in units of 10^{-2} Å^2) are defined by Eq. (d) in Introduction.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{31}	U_{12}
Cs	0	0	0.5	3.19(5)	3.19	2.32(6)	0	0	0
	0	0	0.5	2.44(9)	2.44	1.68(12)	0	0	0
As	0	0	0	2.17(3)	2.17	2.53(6)	0	0	0
	0	0	0	1.50(7)	1.50	2.18(11)	0	0	0
O	0.1455(1)	0.0917(1)	0.1230(1)	3.01(3)	2.99(4)	3.70(4)	−0.76(3)	−1.17(3)	0.47(3)
	0.1456(3)	0.0918(3)	0.1232(3)	2.18(7)	2.24(11)	2.63(6)	−0.41(6)	−0.89(7)	0.11(13)
D	0.1385(4)	0.2192(4)	0.1173(9)	2.7(1)	2.3(3)	2.9(2)	−0.4(2)	−0.2(2)	0.1(1)
	0.1381(10)	0.2184(8)	0.1171(18)	2.3(3)	1.0(8)	1.8(3)	−0.5(5)	−0.5(4)	−0.3(4)

Table 33A-9-002. CsD_2AsO_4 (DCDA). Fractional coordinates at 77 K [81Hay].

	x	y	z
Cs	0	0	0.5123(25)
As	0	0	0
O(1)	0.1194(3)	−0.0281(5)	−0.1254(32)
O(2)	0.0277(3)	0.1196(5)	0.1229(30)
D	−0.0403(10)	0.1797(12)	0.1337(66)

Table 33A-9-003. CsD_2AsO_4 (DCDA). Deuterium bond at Θ_f + 5 K [76Hay]. θ: angle between the line of the two half deuterium positions and the y axis. ϕ: angle between O–O line and the y axis.

O–O in Å	2.531(4)
O–D in Å	1.03(2)
D–D in Å	0.50(2)
θ	14(4)°
ϕ	–0.5(1)°

Table 33A-9-004. CsH_2AsO_4 (CDA). c_{ij} vs. T [79Ani]. c_{ij}: elastic stiffness.

Ultrasonic measurements [$\cdot 10^{10}$ N m^{-2}]							Brillouin scattering measurements [$\cdot 10^{10}$ N m^{-2}]			
T [K]	c_{11}	c_{33}	c_{44}	c_{66}	c_{12}	c_{13}	c_{11}	c_{33}	c_{66}	$\frac{c_{11}+c_{12}+2c_{66}}{2}$
293	5.158	3.988	0.666	0.17	0.056	1.329	5.161	4.01	0.176	2.785
273	5.201	4.018	0.668	0.17	0.043	1.327	5.2	4.04	0.173	2.8
253	5.241	4.071	0.672	0.169	0.019	1.324	5.234	4.08	0.171	2.798
233	5.284	4.113	0.674	0.165	0.016	1.321	5.271	4.1	0.167	2.81
213	5.325	4.154	0.677	0.154	0.009	1.325	5.31	4.16	0.161	2.82
192	5.368	4.195	0.68	0.137	0.006	1.322	5.345	4.19	0.143	2.823
183	5.392	4.214	0.681	0.122	0.014	1.316	5.41	4.22	0.126	2.84
173	5.414	4.238	0.682	0.009	−0.012	1.319	5.41	4.24	0.101	2.805
168	5.425	4.247	0.683	0.08	−0.025	1.296	5.42	4.25	0.086	2.79
163	5.436	4.257	0.684	0.056	−0.03	1.253	5.43	4.26	0.06	2.776
161	5.439	4.26	0.684	0.042	−0.061	1.238	5.43	4.26	0.046	2.74
160	5.441	4.26	0.684	0.037	−0.067	1.222	5.436	4.264	0.04	2.72
159	5.444	4.26	0.685	0.031	−0.07	1.204	5.44	4.264	0.034	2.71
158	5.439	4.262	0.685	0.027	−0.077	1.182	5.44	4.261	0.03	2.705
157	5.436	4.262	0.685	0.024	−0.083	1.152	5.435	4.26	0.026	2.697
156	5.422	4.012	0.679	0.02	−0.09	1.13	5.41	4.2	0.022	2.672
155.8	5.047	3.652	0.677	0.018	−0.097	1.025	5.15	3.67	0.02	2.54

Table 33A-9-005. CsH_2AsO_4 (CDA). Ordinary (n_o) and extraordinary (n_e) refractive indices with respect to air [87Kir]. T = 33.0(4) °C. IF: narrow-band interference filter.

λ [Å]	Source	n_o	n_e
4046.56	Hg	1.59003	1.56669
4358.33	Hg	1.58440	1.56159
4678.15	Cd	1.57987	1.55744
4799.91	Cd	1.57837	1.56612
5085.82	Cd	1.57535	1.55338
5460.74	Hg	1.57206	1.55052
5893.0	Na	1.56894	1.54776
6438.47	Cd	1.56568	1.54502
7800.27	Rb	1.55981	1.54060
7947.60	Rb	1.55931	1.54016
8521.13	Cs	1.55735	1.53892
8943.46	Cs	1.55610	1.53810
10640.00	Xe + IF	1.55148	1.53564

Table 33A-9-006. CsD_2AsO_4 (DCDA). Ordinary (n_o) and extraordinary (n_e) refractive indices with respect to air [87Kir]. T = 33.0(4) °C. IF: narrow-band interference filter.

λ [Å]	Source	n_o	n_e
4046.56	Hg	1.58529	1.56464
4358.33	Hg	1.57990	1.55954
4678.15	Cd	1.57562	1.55553
4799.91	Cd	1.57419	1.55421
5085.82	Cd	1.57122	1.55148
5460.74	Hg	1.56801	1.54856
5893.0	Na	1.56512	1.54593
6438.47	Cd	1.56218	1.54330
7800.27	Rb	1.55701	1.53896
7947.60	Rb	1.55646	1.53854
8521.13	Cs	1.55476	1.53735
8943.46	Cs	1.55371	1.53652
10640.00	Xe + IF	1.54995	1.53413

Table 33A-9-007. $CsH_{2(1-x)}D_{2x}AsO_4$ (x = 0.60). n_o, n_e vs. λ at RT [80Vlo].

λ [nm]	n_o	n_e
365.0	1.5920	1.5685
404.7	1.5855	1.5630
407.8	1.5840	1.5620
435.8	1.5805	1.5580
546.1	1.5690	1.5490
578.0	1.5665	1.5470
632.7	1.5610	1.5445
1014.0	1.5485	1.5345
1152.3	1.5455	1.5325

Table 33A-9-008. CsH_2AsO_4 (CDA), CsD_2AsO_4 (DCDA). Electrooptic constant r_{63}^T of free crystal vs. λ [91Mac]. T = RT.

λ [µm]	r_{63}^T [$\cdot 10^{-12}$ m V^{-1}]	
	CDA	DCDA
0.325	14.6	–
0.340	15.1	–
0.355	16.1	24.9
0.370	16.9	26.5
0.385	17.1	28.2
0.400	17.2	28.3
0.430	17.2	28.4
0.500	17.2	28.6
0.540	17.4	28.7
0.630	17.5	28.9
0.800	17.6	29.1
1.000	17.8	29.2

Table 33A-9-009. CsH_2AsO_4 (CDA). ^{133}Cs quadrupole coupling tensor components in the crystal field fixed $X(a)$, $Y(b)$, $Z(c)$ system [69Gup]. A and B are two physically non-equivalent Cs sites.

T		$eQ\phi_{zz}/h$	$eQ\phi_{yy}/h$	$eQ\phi_{xx}/h$
[K]		[kHz]		
128	A	359(10)	–359(10)	0
	B	359(10)	0	–359(10)
300		359(10)	–179.5(50)	–179.5(50)

Table 33A-9-010. CsH_2AsO_4 (CDA), CsD_2AsO_4 (DCDA). Superhyperfine (shf) couplings for AsO_4^{4-} determined by ENDOR [88Kah]. $\boldsymbol{H} \parallel \boldsymbol{c}$.

Nucleus	shf couplings [MHz] CDA 124 K	 DCDA 110 K
Cs (nearest)	+41.88	+42.01
Cs (second-nearest)	+9.12	+9.08
Cs (third-nearest)	+5.14	+5.04
H (close, two)	–24.7	
H (far, two)	–3.2	